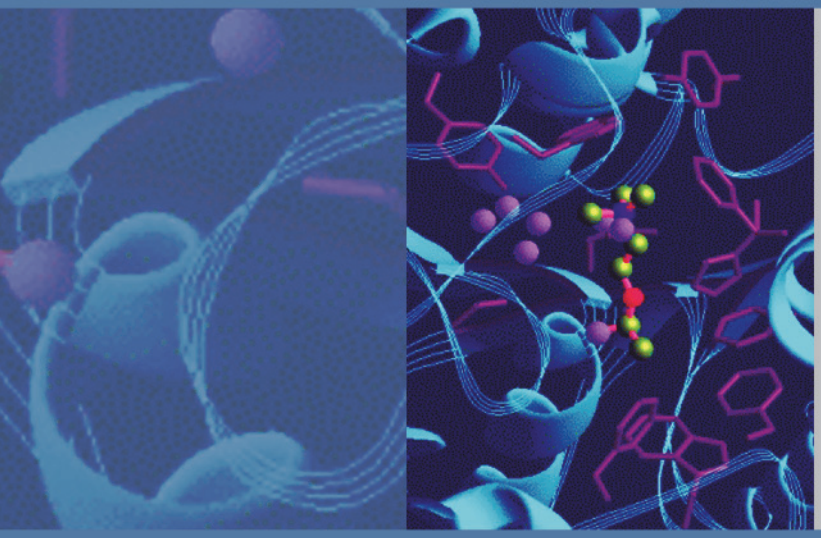

Thermo

Xcalibur

Versions 2.1–2.3

Creating and Searching Libraries User Guide

XCALI-97210 Revision E August 2012

DOCUMENTATION SURVEY

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Preface

The Thermo Xcalibur™ mass spectrometry data system includes all the software needed to create, search, and edit libraries. This guide describes:

- How to create and edit custom libraries for MS, MS/MS, or MSn spectra
- How to manage multiple libraries
- How to search multiple libraries

To provide us with comments about this document, please click the link below. Thank you in advance for your help.

Related Documentation

Thermo Fisher Scientific provides these documents for the Xcalibur data system:

- *Xcalibur Getting Started Guide for Quantitative Analysis*
- *Xcalibur Data Acquisition and Processing User Guide*
- *Xcalibur Quantitative Analysis User Guide*
- *Xcalibur Qualitative Analysis User Guide*
- *Xcalibur Creating and Searching Libraries User Guide*
- *XReport User Guide*
- Help from within the software

Safety and Special Notices

Make sure you follow the precautionary statements presented in this guide. The safety and other special notices appear in boxes.

Safety and special notices include the following:

CAUTION Highlights hazards to humans, property, or the environment. Each CAUTION notice is accompanied by an appropriate CAUTION symbol.

IMPORTANT Highlights information necessary to prevent damage to software, loss of data, or invalid test results; or may contain information that is critical for optimal performance of the system.

Note Highlights information of general interest.

Tip Highlights helpful information that can make a task easier.

Contacting Us

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❖ To contact Technical Support

Phone	800-532-4752
Fax	561-688-8736
E-mail	us.techsupport.analyze@thermofisher.com
Knowledge base	www.thermokb.com

Find software updates and utilities to download at mssupport.thermo.com.

❖ To contact Customer Service for ordering information

Phone	800-532-4752
Fax	561-688-8731
E-mail	us.customer-support.analyze@thermofisher.com
Web site	www.thermo.com/ms

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Go to www.thermoscientific.com/wps/portal/ts/contactus.

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Go to mssupport.thermo.com, agree to the Terms and Conditions, and then click **Customer Manuals** in the left margin of the window.

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- Send an e-mail message to the Technical Publications Editor at techpubs-lcms@thermofisher.com.

Overview of Library Browser

This chapter gives a brief overview of Library Browser, describes how to use data exported from Qual Browser, and describes how to build and maintain a user library.

Contents

- Library Browser Process Overview
- About Library Browser
- Library Browser Windows

Use Xcalibur Library Browser to do these tasks:

- Create spectral libraries, including MS/MS fragmentation libraries.
- Use the Library Browser to run automatic, post-acquisition library searches on MS/MS fragmentation spectra.
- Run searches directly from the Qual Browser in the data system or automatically by batch processing data files in the Sequence Setup window using a qualitative processing method.

"Library Browser Process Overview" on page 2 summarizes the steps for creating, editing, and searching custom libraries and printing reports of the results.

This chapter also provides information about how to choose a peak detection algorithm for the Xcalibur data system to use when performing library searches.

Note Throughout this guide, the term *Library Browser* is used synonymously with the term *NIST MS Search* (National Institute of Standards and Technology Mass Spectral Search Program and Library System) to refer to the NIST MS Search desktop.

Library Browser Process Overview

Figure 1 provides a summary of the steps you perform to create, edit, and search libraries and to print reports using the Xcalibur data system.

When using the Library Browser, create a custom user library of MS/MS or MS^n spectra, one entry at a time. To include a spectrum in a library entry, display a qualitative .raw file data in Qual Browser. Then, in Qual Browser, you can enhance a spectrum by averaging several scans and by subtracting background scans.

After enhancing the spectrum, you can export the spectrum to Library Browser. See "Adding Spectra to a User Library" on page 29 for more information on this process.

After exporting the spectrum to Library Browser, you can edit the spectrum information. For example, you can change the name of the entry or specify the molecular weight or the CAS (Chemical Abstract Service) registry number. You can even attach a chemical structure to the library entry or select which mass-to-charge ratios to include. See "Managing Libraries" on page 25 for more information.

IMPORTANT For MS/MS and MS^n spectra, however, do not delete any of the masses that the data system detects because the presence of a particular mass-to-charge ratio, rather than its intensity, is essential to identifying a compound.

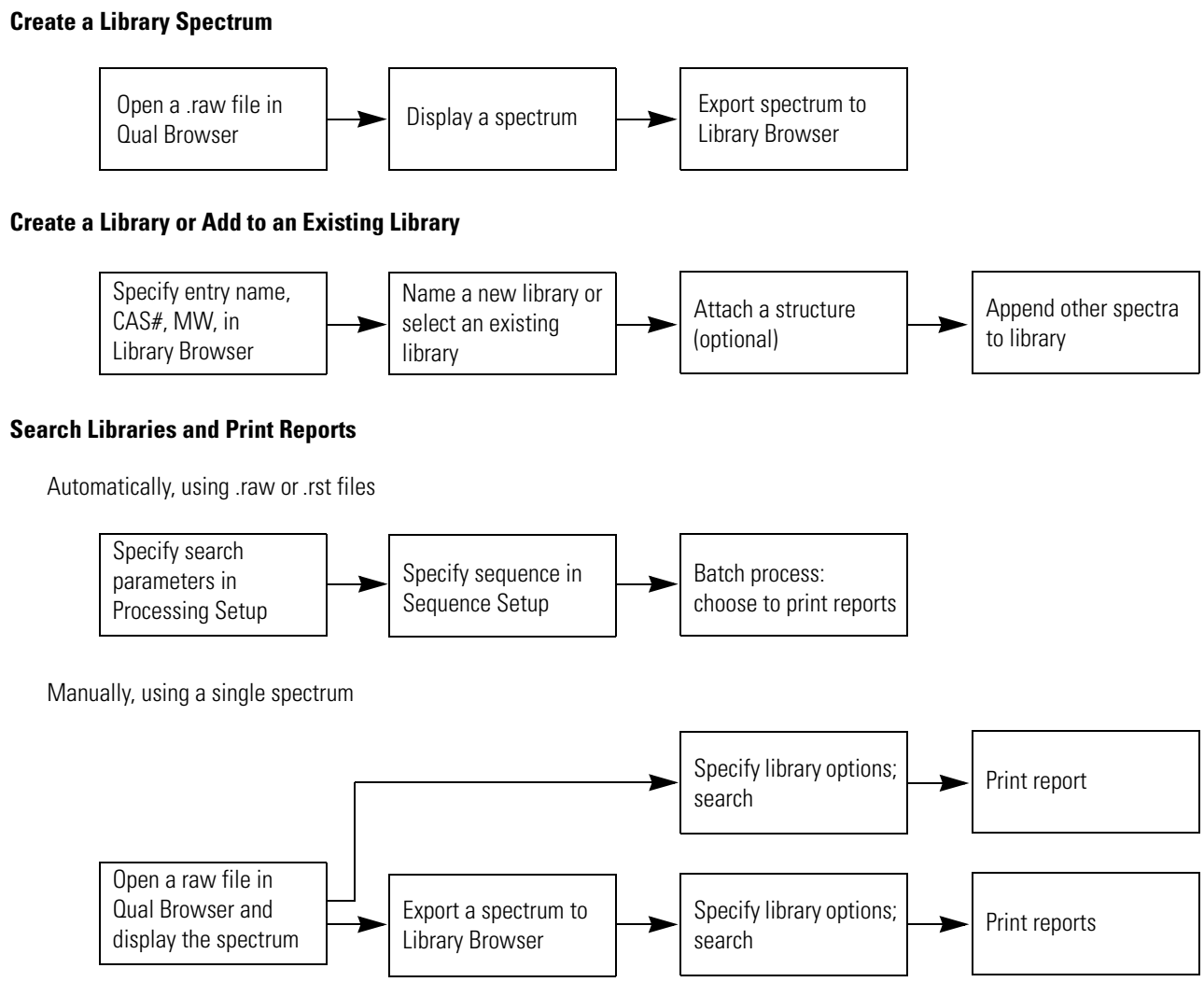
Finally, the Xcalibur data system provides three ways to search libraries and print custom reports:

- Automatically, by using raw (.raw) or result (.rst) files in Sequence Setup (See "Setting Up to Search Libraries Automatically" on page 64 for more information.)
- Manually, by using a single spectrum in Qual Browser (See "Initiating a Library Search from Qual Browser" on page 77 for more information.)
- Manually, by using a single spectrum exported to Library Browser (See "Searching a Library Using Library Browser" on page 80 for more information.)

You can use the Qual view options in the Processing Setup window to specify a processing method to print reports automatically. Then reference this processing method to specify a sequence of files in Sequence Setup. When you process a sequence, the data system prints the reports. Refer to the *Acquisition and Processing User Guide* for more information about using Processing and Sequence Setup. You can also create processing settings to automatically add spectra to the library.

If you manually search for search results that match a single spectrum, print the results by using the **File > Print** command in Qual Browser or in Library Browser.

Figure 1. Library Browser process overview


Create a Library Spectrum
Open a .raw file in Qual Browser
Display a spectrum
Export spectrum to Library Browser
Create a Library or Add to an Existing Library
Specify entry name, CAS#, MW, in Library Browser
Name a new library or select an existing library
Attach a structure (optional)
Append other spectra to library
Search Libraries and Print Reports
Automatically, using .raw or .rst files
Specify search parameters in Processing Setup
Specify sequence in Sequence Setup
Batch process: choose to print reports
Manually, using a single spectrum
Specify library options; search
Print report
Open a raw file in Qual Browser and display the spectrum
Export a spectrum to Library Browser
Specify library options; search
Print reports

About Library Browser

The Xcalibur data system uses the NIST (National Institute of Standards and Technology) Mass Spectral Search Program and Library System. This system contains up to three different libraries:

- The 2000 version of the NIST/EPA/NIH Mass Spectral Library containing over 147000 compounds (optional)
- The NIST/EPA/NIH Mass Spectral Selected Replicates Library of 27750 spectra (optional)
- A default user library, NISTDEMO

The NIST libraries give access to

- An extensive collection of chemical names
- Chemical Abstracts Service (CAS) registry numbers
- Molecular formulas and weights
- Chemical structures

You can create user libraries using spectra

- Exported from Qual Browser
- Exported automatically by a processing method
- From other sources including text files

The program permits searches in many different ways:

- Find reference spectra most closely matching a submitted spectrum.
- Locate spectra or compounds having certain specified characteristics (for example, the abundance of certain peaks).
- Display the mass spectra of selected molecules.

Library Browser Windows

The Library Browser contains five main windows with tabs at the bottom of the window:

- Library Search Window
- Other Search Window
- Name Search Window
- Compare Window
- Librarian Window

A description of each of these windows follows.

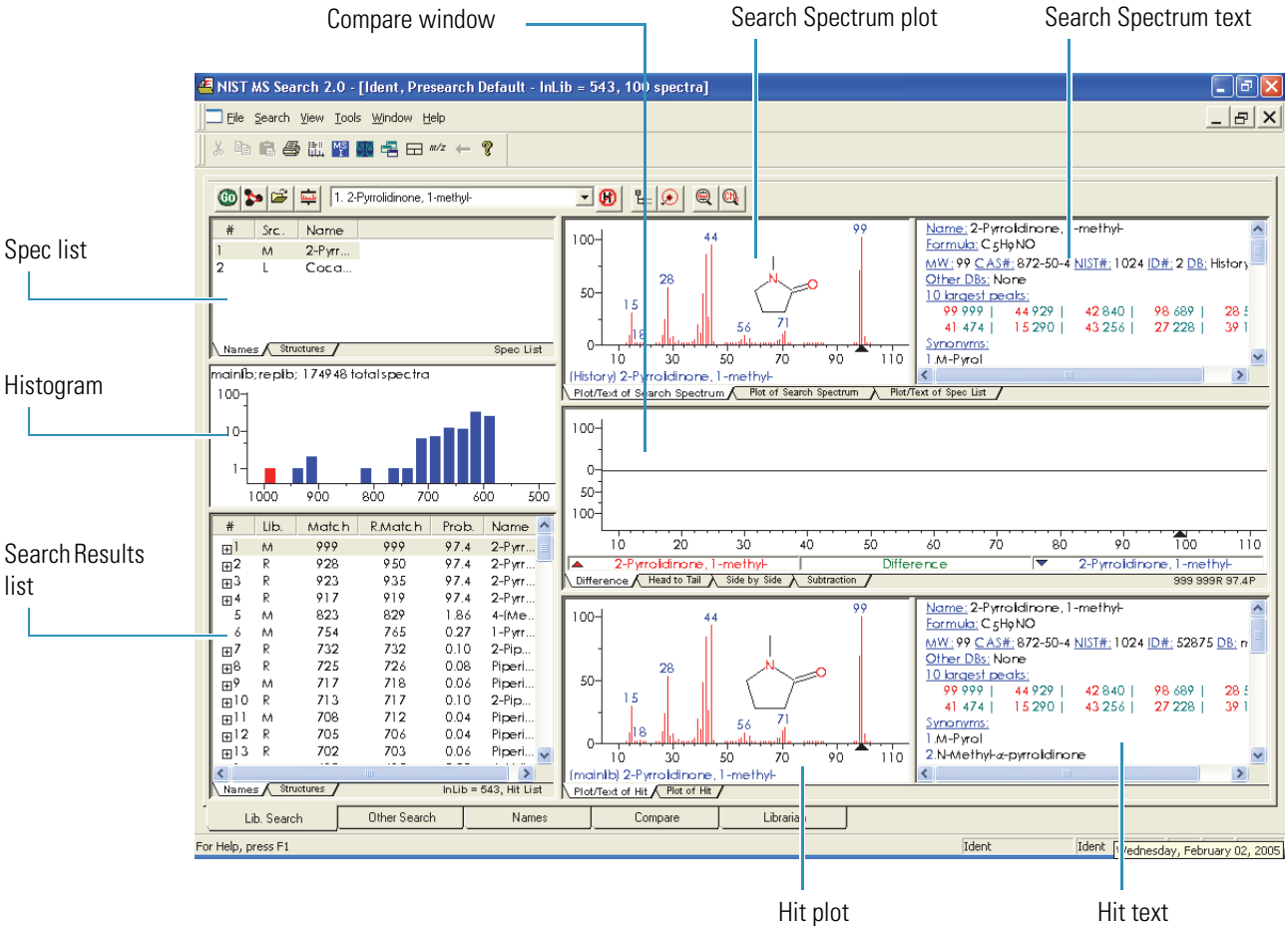
To display a specific window, click the appropriate tab at the bottom of the screen.

Library Search Window

The Library Search window of the Library Browser (see Figure 2) features eight panes:

Spec list	A "scratch pad" for storage of imported spectra and database spectra of interest
Histogram	A graphical display of the number of matches as a function of the match factor Click a bar to change the information displayed in the other windows.
Search results (Hit list)	A list of compounds in the database with spectra that are similar to the unknown
Plot of Search Spectrum	The plot of the spectrum being investigated
Text of Search Spectrum	Text about the spectrum being investigated
Difference (Compare Result)	A graphical display of peaks from the first (often upper) spectrum and the second (often lower) spectrum along with the difference.
Plot of Hit	The spectrum of a search result
Hit Text Information	Text concerning an item from the search results

Figure 2. Library Search window



Using the Spec List

The Library Browser stores spectra in the Spec List pane of the Library Search window when you do either of the following:

- Export spectra from Qual Browser
- Import spectra from other sources using the **File > Open** command
- Get a spectrum from a library

The Browser identifies the origin of each Spec List entry with an initial letter:

(T) Spectra that came directly from a text file such as that exported by Qual Browser

(E) Spectra created with the Edit or New buttons in the User Library Manager window

(M) Spectra from the NIST/EPA/NIH Main library

(R) Spectra from the NIST/EPA/NIH Replicates library

(U) Spectra from a user library

❖ To submit a Spec List spectrum to a Library Browser search

1. Set the Library Search options. See "Customizing a Search" on page 50.
2. Double-click the spectrum name.

The Browser displays all search results in the search results (Hit List) pane (see below).

Comparing a Spec List Spectrum in the Compare Pane

To transfer a Spec List entry to the Compare window, double-click the entry. See "Displaying Spectra in the Compare Window" on page 10.

Using the Hit List

The Hit List displays a list of library spectra that match the unknown spectrum from highest to lowest match in the Library Search window. Each search result is listed with its order number, forward and reverse matching factors, and a library identifier:

- (M) for the Main NIST library
- (R) for the Replicates library
- (U) for a user library

Click a name from the search results to display its spectrum and structure in the Plot pane and to display text describing the hit in the Text pane. The spectrum also appears in the Compare window.

The Plot and Text Panes

The Plot panes display the following:

- The full spectrum or expanded views of a selected *m/z* range
- The compound structure (if available)

The Text panes display the following:

- Compound Information: name, formula, molecular weight, CAS number, NIST number, ID number, and search library
- The ten largest peaks in the mass spectrum
- Synonyms or alternate names used in the library

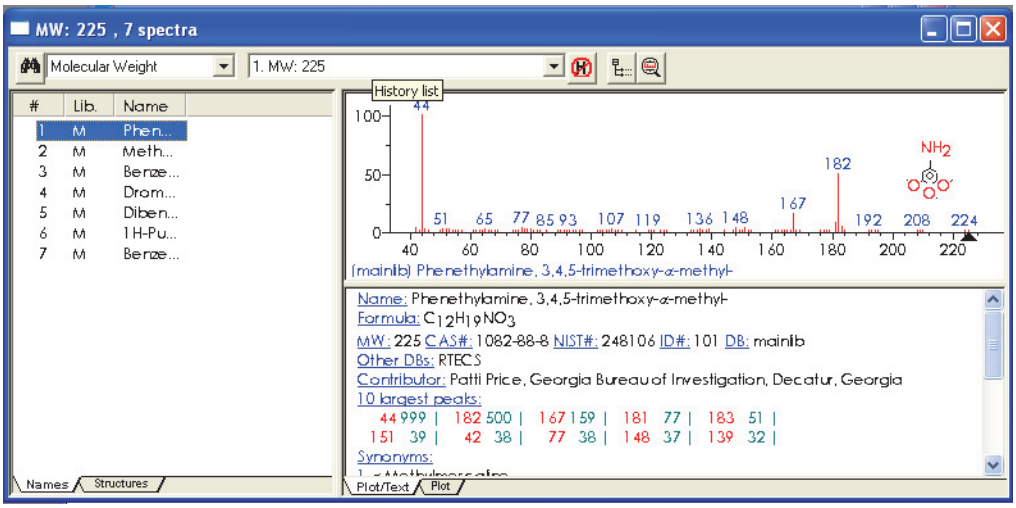
Other Search Window

The Other Search window of the Library Browser (see Figure 3) can carry out searches based on the following:

- Formula
- ID number
- Molecular weight
- Any peaks
- CAS Registry number
- Sequential method
- NIST library number

Launch these searches by selecting the appropriate option from the Search Type list in the top left corner of the window or use the appropriate command from the Search menu. For more information about modifying searches, see "Searching Libraries" on page 49.

Figure 3. Other Search window


MW: 225 , 7 spectra
Molecular Weight
1. MW: 225
History list
Lib. Name
1 M Phen...
2 M Meth...
3 M Benze...
4 M Drom...
5 M Diben...
6 M 1H-Pu...
7 M Benze...
Names Structures
(mainlib) Phenethylamine, 3,4,5-trimethoxy-α-methyl-
Name: Phenethylamine, 3,4,5-trimethoxy-α-methyl-
Formula: C12H19NO3
MW: 225 CAS#: 1082-88-8 NIST#: 248106 ID#: 101 DB: mainlib
Other DBs: RTECS
Contributor: Patti Price, Georgia Bureau of Investigation, Decatur, Georgia
10 largest peaks:
44 999 | 182 500 | 167 159 | 181 77 | 183 51 |
151 39 | 42 38 | 77 38 | 148 37 | 139 32 |
Synonyms:
Plot/Text Plot

Name Search Window

❖ To search a NIST library for a compound name or a text fragment

1. In the Name Search window, type a search name into the box in the top left corner of the window, for example, PACETO (see Figure 4).

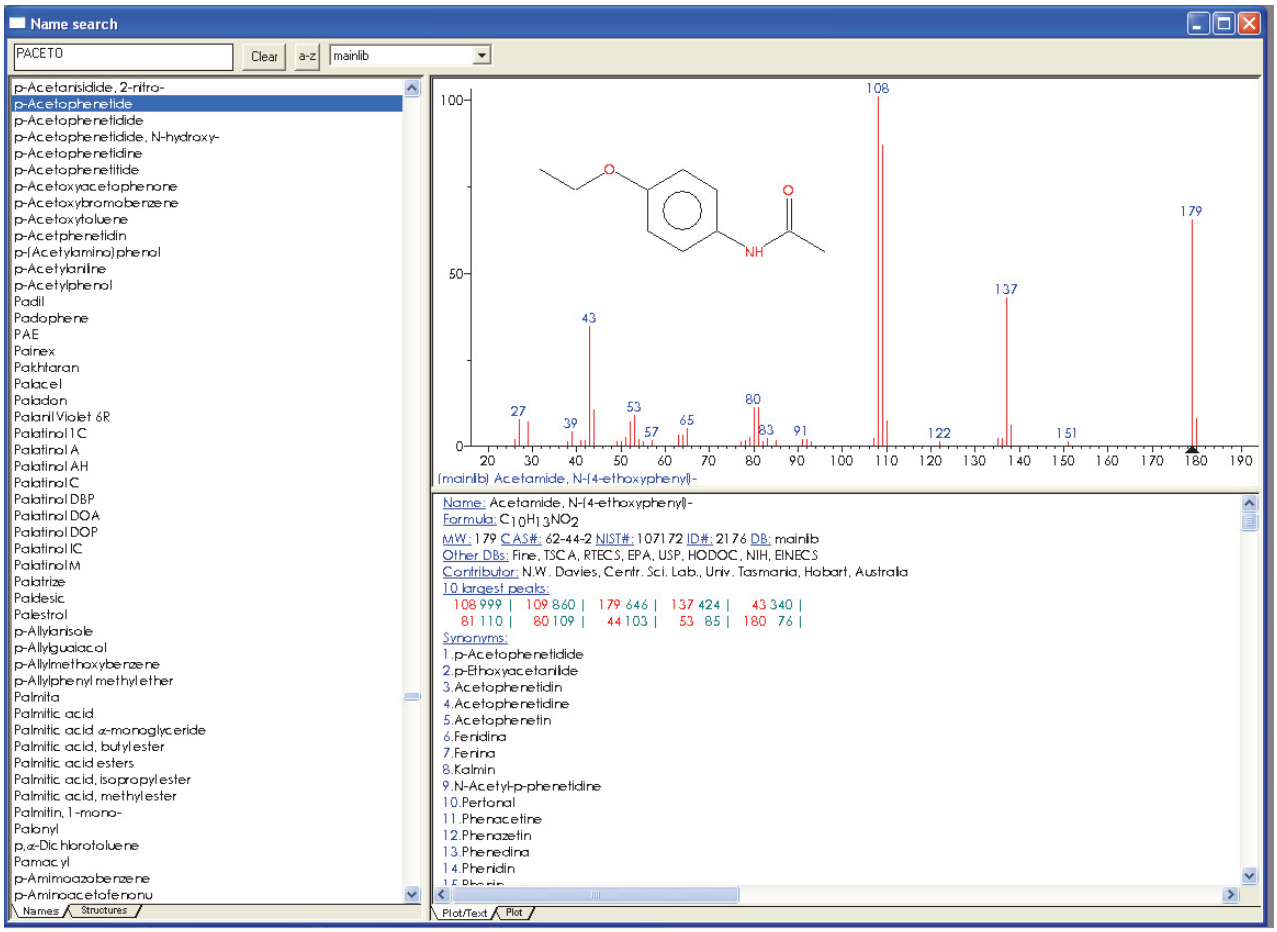
   The Xcalibur data system displays spectrum, structure, and text information in panes in the Name Search window.

2. Right-click an entry. Choose **Library Search** from the shortcut menu.

   The Browser loads details of the compound into the Compare window and the Plot, Text, Compare, and Hit List panes of the Library Search window.

   The default name search mode accepts both alphabetic (a–z) and numeric (0–9) characters. Punctuation and spacing are ignored (for example, *1-butene* is equivalent to *1butene*). Greek characters must be spelled out (for example, *alpha*).

Figure 4. Name search window

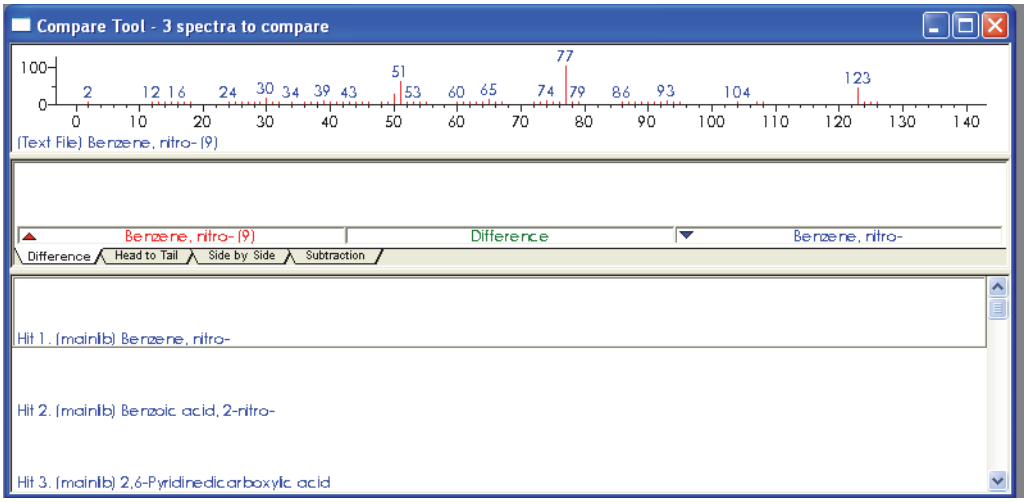


With the **a to z only, no prefix** option selected, the Browser accepts only alphabetic characters and ignores common prefixes (for example, cis, trans, dl, di, and tri), numbers, and Greek characters. In this mode, typing butene finds 1-butene and cis 2-butene.

Compare Window

The Compare window is used for the comparison of spectra only—it has no searching capabilities. It supports comparison of any set of spectra and, unlike the Library search window, it can show multiple spectra. There are three panes in the Compare window. The top pane is a plot of the spectral display, the middle pane is a standard difference display pane, and the bottom pane displays multiple spectra from the Hit List.

Figure 5. Compare window



The Compare window uses the standard Difference Display options as follows:

Difference	Shows peaks from the first (often upper) spectrum and second (often lower) spectrum along with the difference.
Head to Tail	Shows only the two spectra being compared. The first spectrum points upward, the second spectrum points downward from a common axis.
Side by Side	Shows only the two spectra displayed next to each other.
Subtraction	Creates a spectrum derived by subtracting the second spectrum from the first.

Displaying Spectra in the Compare Window

❖ To add spectra to the top pane

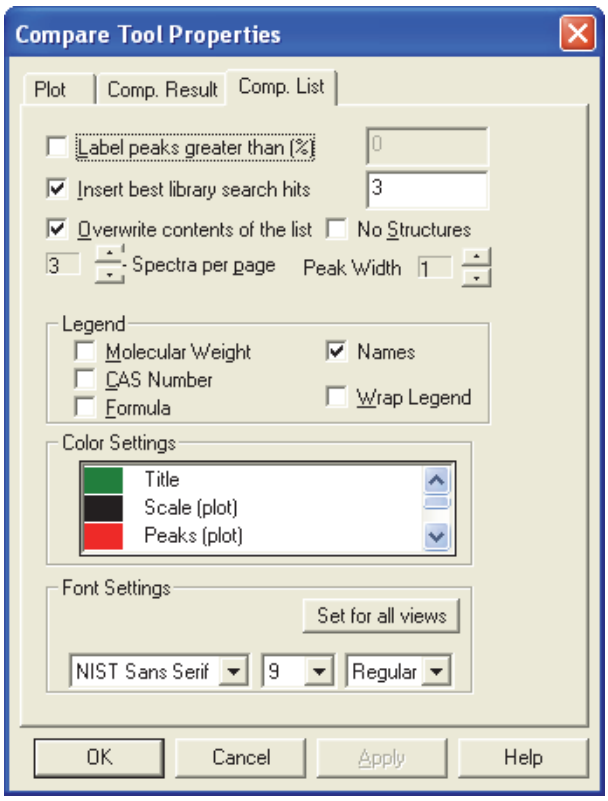
1. Double-click an entry in the Spec List of the Library Search window or select an entry in either the Spec List or the Hit List of the Library Search window.
2. Right-click the entry and choose **Copy** from the shortcut menu.
3. To paste the desired spectra in the top pane, go to the Compare window and use the **Paste** command on the shortcut menu.

Formatting the Compare Window

❖ To format the compare window

Right-click in the pane and choose **Properties** from the shortcut menu. The Compare Tool Properties dialog box opens.

Figure 6. Compare Tool Properties dialog box



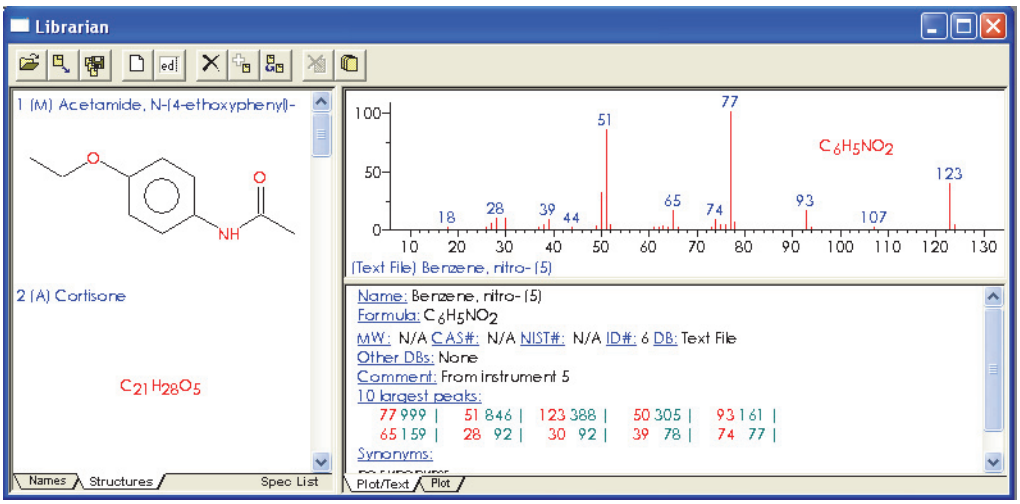
You can use the Compare Tool Properties dialog box to change parameters for these options.

- Plot page: Specify plot view parameters.
- Comp. Result: Specify compare view parameters.
- Comp. List: Specify compare list parameters:
  - Insert best library search hits: Automatically inserts the number of hits specified from the top of the hit list to the compare list.
  - Overwrite contents of the list: automatically overwrites the current contents of the list with new information. If you do not select this option, data is added to the top of the compare list.
  - No structures: puts no structures on the compare window.
  - Spectra per page: specifies the number of structures from the compare list that are shown below the compare window.

Librarian Window

The Librarian window is the User Library manager for the Library Browser. Use it to create User Libraries and to add spectrum files and compound information to them. Also use the Librarian window to create, save, and edit text files, save mass spectra, and edit compound ID information.

Figure 7. Librarian window


Librarian
1 (M) Acetamide, N-(4-ethoxyphenyl)-
2 (A) Cortisone
C21 H28O5
Names
Structures
Spec List
(Text File) Benzene, nitro- (5)
Name: Benzene, nitro- (5)
Formula: C6H5NO2
MW: N/A CAS#: N/A NIST#: N/A ID#: 6 DB: Text File
Other DBs: None
Comment: From instrument 5
10 largest peaks:
77 999 | 51 846 | 123 388 | 50 305 | 93 161 |
65 159 | 28 92 | 30 92 | 39 78 | 74 77 |
Synonyms:
Plot/Text
Plot

The Librarian window is divided into three panes:

- A Spec List shows the names of all files under consideration, including structure and formula if available.
- A Plot pane shows the spectrum of a file in the Spec List
- A Text pane displays any detailed text on the selected file in the Spec List

❖ To delete a spectrum

Click to remove a spectrum and any associated library from the list without saving them anywhere.

❖ To add a spectrum

Click to add the highlighted spectrum on the list to a designated User library.

❖ To move a spectrum

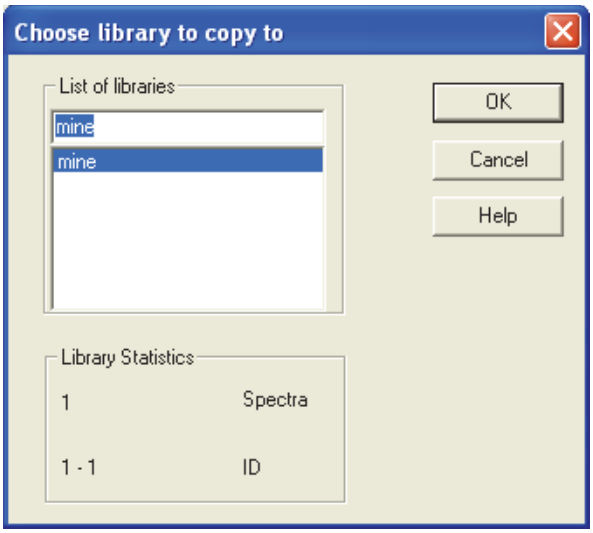
Click to remove the highlighted spectrum from the list and put it into a designated user library.

❖ To delete a user library

Click to remove an entire user library.

Click the **Add**, **Move**, and **DelLib** buttons to open a dialog box listing the available user libraries. Select the library required for the command. When adding or moving a spectrum, type a new user library name, if required.

Figure 8. Chose library to copy to dialog box



The dialog box also features buttons for managing individual library entries:

Click **New** to create a new library entry.

Click **Edit** to change a current library entry in the Spectrum Information dialog box.

Adding a Spectrum to a Library

To create a library entry with MS or MS/MS (or MS^n) spectral data, use the Qual Browser window.

The procedure in this section uses steroid data. The Xcalibur data system stores the raw data files in the C:\Xcalibur\examples\data directory.

To manually create a library entry, complete the tasks detailed below:

Contents

- Opening a Raw Data File in Qual Browser
- Viewing a Spectrum in Qual Browser
- Working with Background Spectra
- Exporting Spectra from the Xcalibur Data System

Opening a Raw Data File in Qual Browser

To view raw data, use the Qual Browser window. Open a data file to expand the Qual Browser menu bar.

❖ **To display the raw data of a steroids data file**

1. To display the Xcalibur Home Page from your computer desktop, double-click or choose **Start > Programs > Thermo Xcalibur > Xcalibur** on the computer desktop.
2. To display the Qual Browser window, click on the Xcalibur Home Page.
3. Choose **File > Open** or click in the toolbar. The Open Raw File dialog box opens.
4. Browse to the location of the raw file and select the file.
5. Click **Open**. The chromatogram and first mass spectrum for this data file appear (see Figure 9).

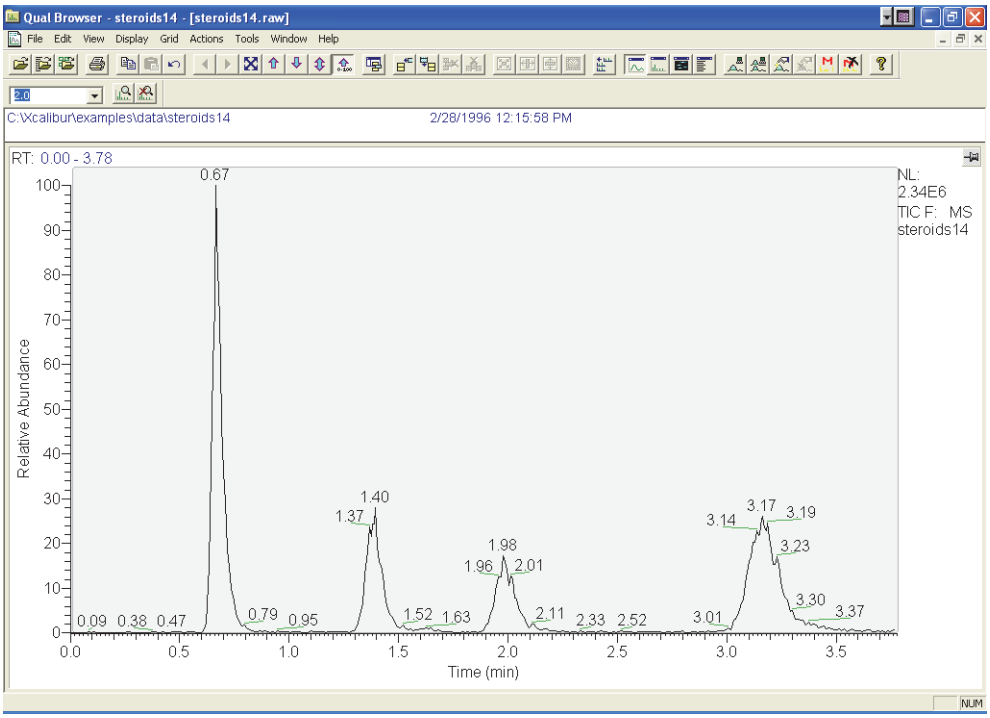
Viewing a Spectrum in Qual Browser

To view a mass spectrum, use the interactive cells of the Qual Browser window.

❖ To display a mass spectrum of the raw data in a window containing four cells

1. Confirm that the data system displays a Chromatogram view similar to Figure 9. If you cannot see the chromatogram view, do the following:
   a. Select a cell. The application shows both the chromatogram and spectrum by default.
   b. Choose **View Spectrum**.
   c. Choose **Grid > Delete > All Cells** to remove the chromatogram.
   d. Select **View** and clear all entries except Spectrum to expand the chromatogram to the full size of the Qual Browser window.
   e. To enlarge the window display area, click ☐ in the upper right corner of the window.

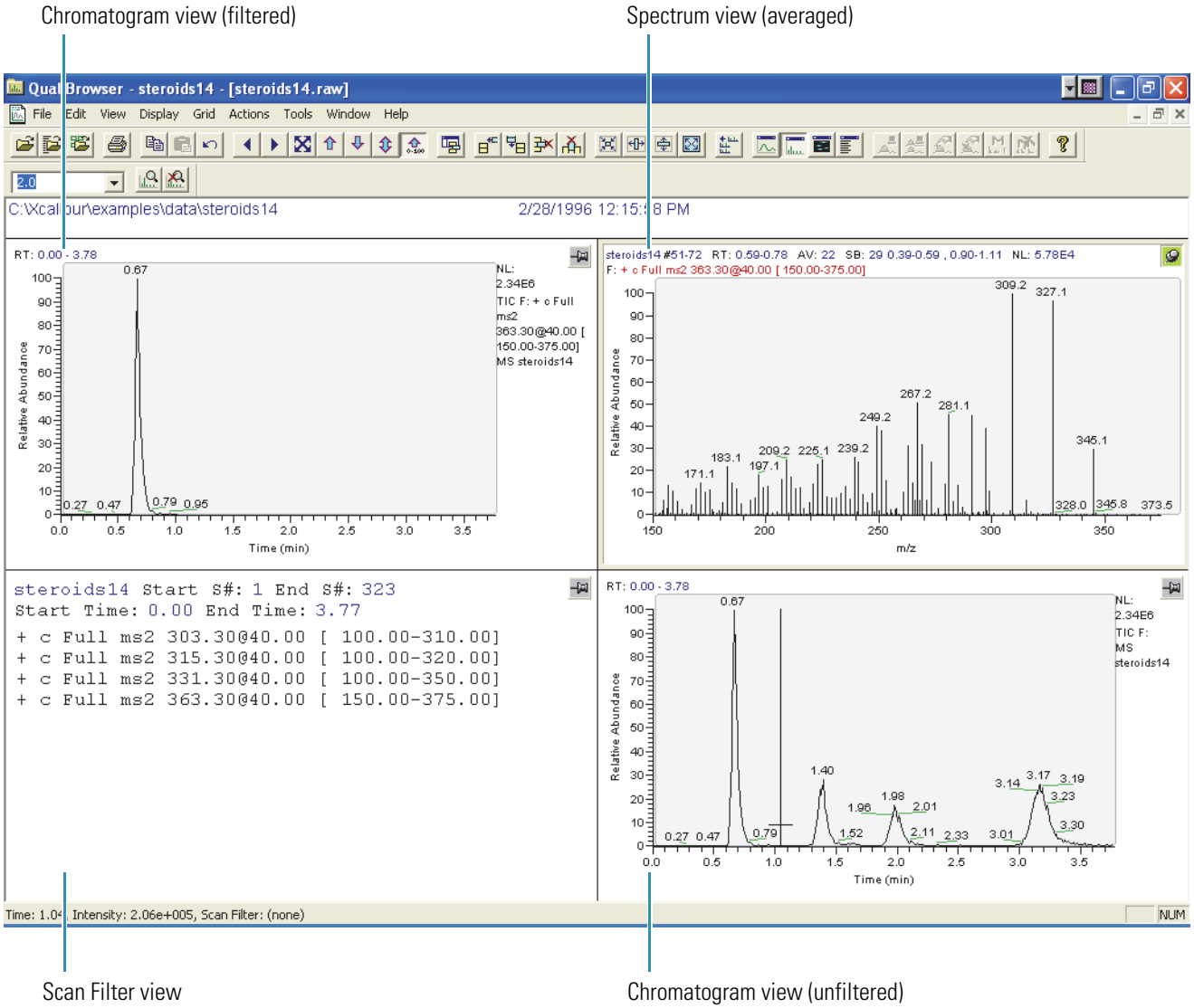
Figure 9. Qual Browser window, showing the Chromatogram view of the raw file



2. Open cells to display the raw data in a grid of four cells (as shown in Figure 10):
   a. To display two cells in the window, choose **Grid > Insert Cells > Left**.
   b. To display four cells in the window, choose **Grid > Insert Cells > Below**.

Figure 10 shows the following views (clockwise from lower left): Scan Filter view, (filtered) Chromatogram view, (averaged) Spectrum view, and (unfiltered) Chromatogram view.

Figure 10. Qual Browser window


Chromatogram view (filtered)
Spectrum view (averaged)
Qual Browser - steroids14 - [steroids14.raw]
File Edit View Display Grid Actions Tools Window Help
C:\Xcalibur\examples\data\steroids14
2/28/1996 12:15:38 PM
RT: 0.00 - 3.78
Relative Abundance
Time (min)
NL: 2.34E6 TIC F: + c Full ms2 363.30@40.00 [150.00-375.00] MS steroids14
steroids14 #51-72 RT: 0.59-0.78 AV: 22 SB: 29 0.39-0.59 , 0.90-1.11 NL: 5.78E4
F: + c Full ms2 363.30@40.00 [150.00-375.00]
m/z
steroids14 Start S#: 1 End S#: 323
Start Time: 0.00 End Time: 3.77
+ c Full ms2 303.30@40.00 [100.00-310.00]
+ c Full ms2 315.30@40.00 [100.00-320.00]
+ c Full ms2 331.30@40.00 [100.00-350.00]
+ c Full ms2 363.30@40.00 [150.00-375.00]
RT: 0.00 - 3.78
NL: 2.34E6 TIC F: MS steroids14
Time: 1.04 Intensity: 2.06e+005, Scan Filter: (none)
NUM
Scan Filter view
Chromatogram view (unfiltered)

3. To display the scan filter data, click the lower left cell and choose **View > Scan Filters**. The cell lists the filters contained in the total ion current (TIC) chromatogram over a specified time range.

4. To display a mass range chromatogram in the upper left cell

   a. Make a cell active by clicking in the upper right corner.

   b. Click and hold an entry in the list. The data system surrounds the entry with a box and displays a page cursor.

c. Drag the page cursor to the upper left cell and release the mouse button. The application automatically applies the filter and displays the mass range chromatogram.

5. To display an averaged mass spectrum in the upper right cell:
   a. Make a cell active by clicking in the upper right corner.
   b. Display a mass spectrum by choosing **View > Spectrum**.
   c. Click and hold in the upper left cell at a position just to the left of the chromatogram peak.
   d. Drag the cursor horizontally across the peak and release the mouse button. The Xcalibur data system displays a mass spectrum in the upper right cell. This spectrum is the average of the scans in the retention time range that you selected. For example, see the upper right cell in Figure 10.

Working with Background Spectra

This topic explains how to remove spectra from a display so that only essential spectra are there.

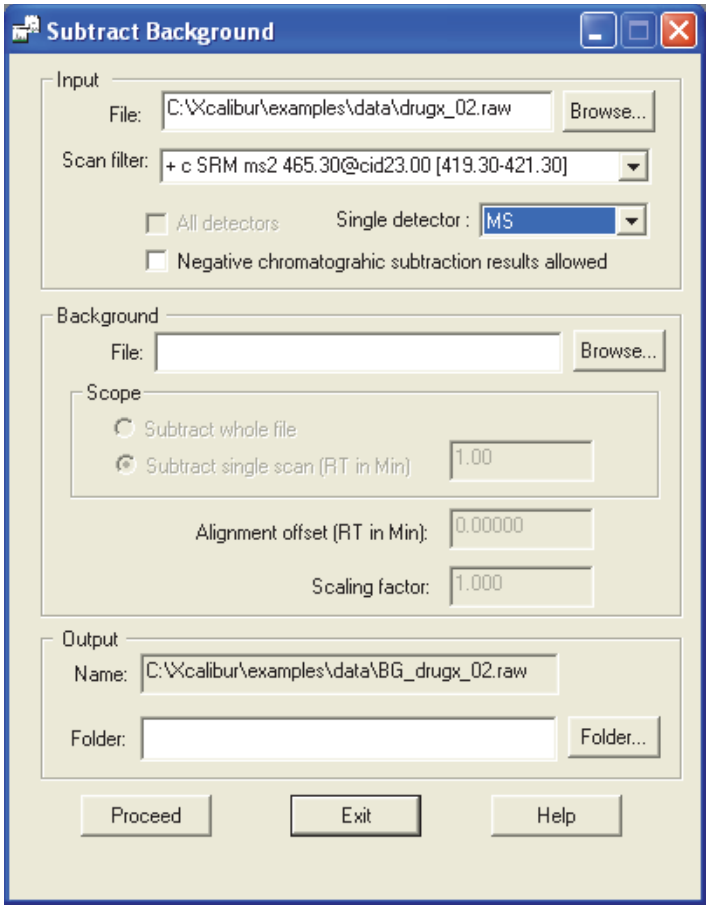
- Using the Subtract Background Tool
- Subtracting Background Spectra

Using the Subtract Background Tool

❖ To change the library search list

1. To open the Subtract Background dialog box, choose **Tools > Background Subtract** from the Qual Browser window.

Figure 11. Subtract Background dialog box



2. To select the input file, type the pathname of the input file in the File box or click **Browse** and locate the file using the Open dialog box.
3. To choose the detector(s), identify data from the required detector source using the Single Detector list. To use all the detectors recorded in the raw file, select the **All Detectors** check box.
4. To choose a scan filter, click the **Filter** arrow to display filter options that are stored in the .raw file. Then, select a filter.
5. To select the background file, type the pathname of the background file in the File box or click **Browse** and locate the file using the Open dialog box.

6. Select the scope of the subtract background file operation:
   - To subtract the entire background file from the input file, select the **Subtract Whole File** option.
   - To subtract a single scan from the background file from each scan of the input file, select the S**ubtract Single Scan** (RT) option and type the retention time for the scan in the associated box.
7. Specify alignment and scaling:
   - To offset the subtraction of the background file from the input file, type the required offset in the Alignment Offset (RT) box.
   - To scale the subtraction of the background file from the input file, type the required factor in the Scaling Factor box.
8. To specify the location of the output file, type the full path location for the output file in the **Folder** box or click the **Folder** button and browse to the required location.

   The dialog box displays the name of the output file as BG_<Input File> in the Name box.
9. To start the subtract background file operation, click **Process**. The dialog box closes.

   To abandon the file operation and close the dialog box, click **Exit**.

Subtracting Background Spectra

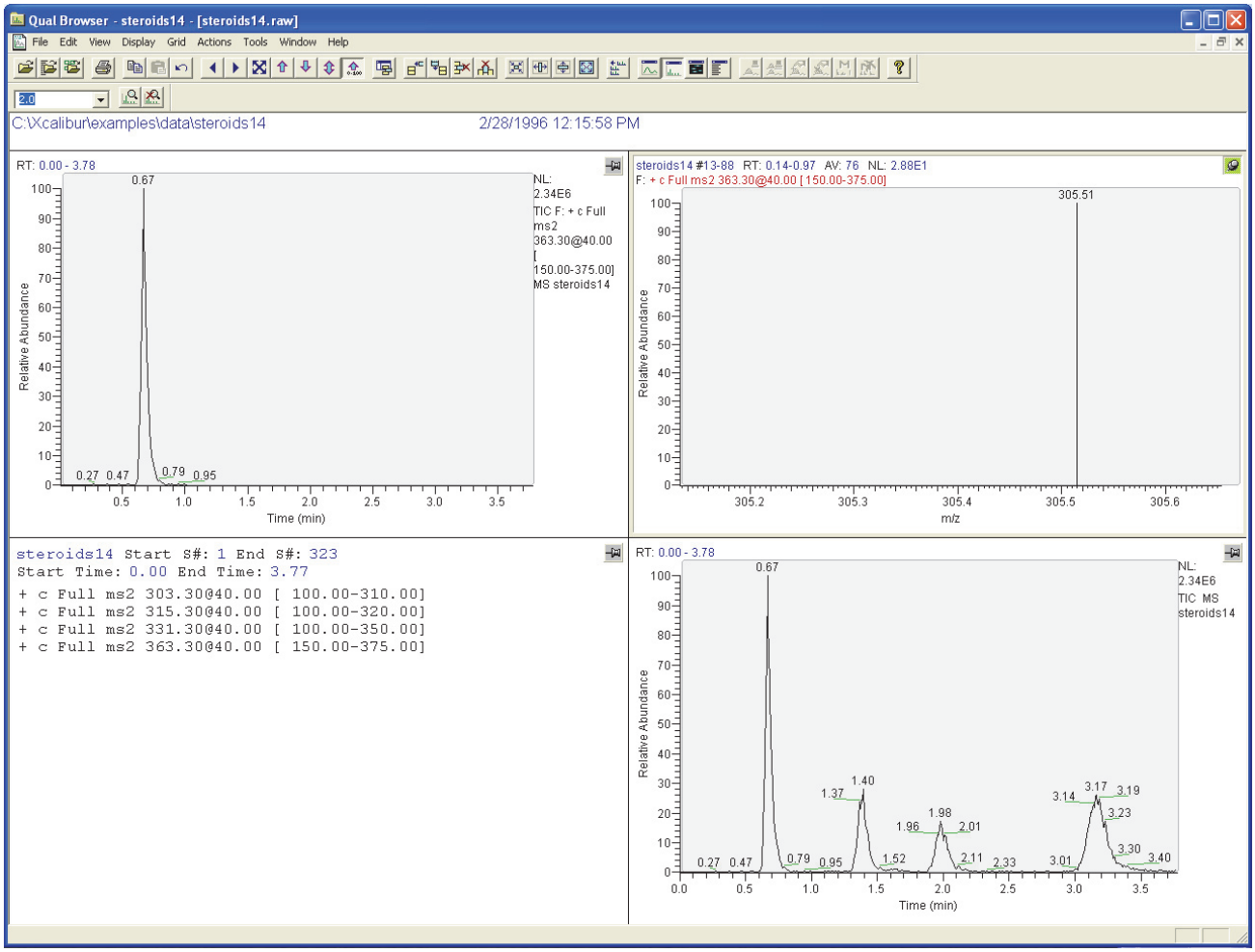
To subtract background spectra, eliminating background peaks from either one range (either side of the chromatogram peak of interest) or two ranges (both sides of the chromatogram peak of interest), use the Chromatogram view.

❖ To select two scan ranges for background subtraction

1. To select a spectrum, click in the upper right corner of the spectrum.
2. Choose **Actions > Subtract Spectra > 2 Ranges** to display the crosshair cursor labeled *-1*.
3. Click and hold on a baseline region in the upper left cell that is close to the chromatographic peak of interest.
4. Drag the cursor away from the peak of interest and across a few scans that are representative of the first scan range to subtract.
5. Release the mouse button to define the first range. The label on the cursor changes to *-2*.
6. Click and hold on a baseline region on the other side of the peak of interest.

7. Drag the cursor away from the peak of interest and across a few scans that are representative of the second scan range to subtract (see Figure 12).

Figure 12. Qual Browser window, showing background subtracted scans in the Spectrum view (upper right)


Qual Browser - steroids14 - [steroids14.raw]
File Edit View Display Grid Actions Tools Window Help
C:\Xcalibur\examples\data\steroids14 2/28/1996 12:15:58 PM
RT: 0.00 - 3.78
NL: 2.34E6 TIC F: + c Full ms2 363.30@40.00 [150.00-375.00] MS steroids14
Relative Abundance
Time (min)
steroids14 #13-88 RT: 0.14-0.97 AV: 76 NL: 2.88E1
F: + c Full ms2 363.30@40.00 [150.00-375.00]
305.51
m/z
steroids14 Start S#: 1 End S#: 323
Start Time: 0.00 End Time: 3.77
+ c Full ms2 303.30@40.00 [100.00-310.00]
+ c Full ms2 315.30@40.00 [100.00-320.00]
+ c Full ms2 331.30@40.00 [100.00-350.00]
+ c Full ms2 363.30@40.00 [150.00-375.00]
RT: 0.00 - 3.78
NL: 2.34E6 TIC MS steroids14

8. To define the second range, release the mouse button.

   When you release the mouse button, the data system subtracts an average of the selected scans and redraws the Spectrum view. The Spectrum view header shows the number of subtracted scans. For example, SB: 12 0.52-0.56, 0.92-0.99 indicates the following:

   - Qual Browser has applied background subtraction to the spectrum by using a 12-scan average.
   - Retention time ranges used in the subtraction are 0.52 to 0.56 min and 0.92 to 0.99 min.

Exporting Spectra from the Xcalibur Data System

To create a library entry for a custom library, export a spectrum from the Spectrum view of Qual Browser to the Library Browser.

To export spectra from the data system to the Library Browser, use one of these methods:

- Exporting Spectra Manually from Qual Browser
- Exporting Spectra Automatically from the Processing Method

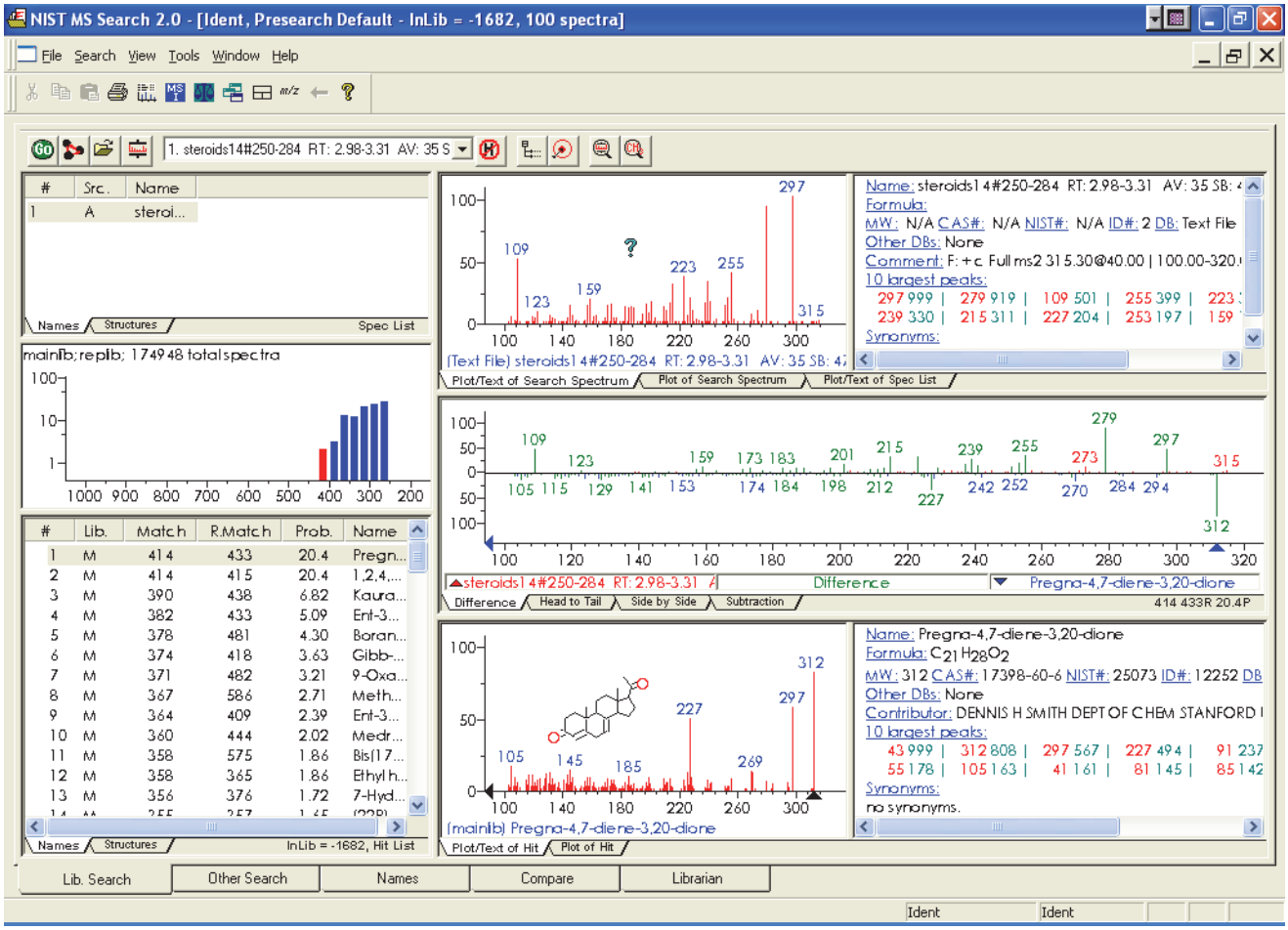
For more information, see "Adding Spectra to a User Library" on page 29.

Exporting Spectra Manually from Qual Browser

❖ **To export the enhanced spectrum to Library Browser**

To export an MS/MS spectrum to the Library Browser, right-click the spectrum view (upper right cell) and choose **Library > Export to Library Browser**. Xcalibur automatically displays the Library Browser (see Figure 13).

Figure 13. Library Search window



The data system converts the mass and intensity data of the spectrum to a text file and copies the file to the Spec List pane. The Qual Browser window stays open. The data system creates the following:

- A copy of the exported spectrum in the Xcalibur\Libspecs folder. The file is given an .msd extension with the same filename as the original data file, although this is truncated to eight characters (8.3 filename format).
- An index file containing details about all exported spectra.
- The data system places the exported spectrum into the Spec List (Spectrum List), and the Library Browser immediately searches the selected libraries for matching spectra if you check the Automation option in the Library Search Property dialog box.

To display the Library Search Property dialog box, choose **Tools > Search Options**.

To display the Automation option check box, click either the **Search** tab or the **Automation** tab. See "Setting Up to Search Libraries Automatically" on page 64.

Exporting Spectra Automatically from the Processing Method

The processing method contains the Append to User Library option to automatically export a spectrum directly into a user library. If the specified library does not exist, the Xcalibur data system creates it.

When a spectrum is added to a user library, it contains the following basic information:

- The complete mass/intensity list
- A name formatted as <filename>#<scannumber> RT: <rt> AV: <av> NL: <nl>
  for example: steroids02#1 RT: 0.01 AV: 1 NL: 2.14E3
- A comment showing the Scan Filter, such as T: + c Full ms2 363.30 [150.00 - 375.00]
- The Mol Weight and CAS Number fields are set to zero.

You might want to modify the basic information or provide the following:

- A chemical formula
- A list of synonyms
- The molecular weight
- The CAS number
- A chemical structure (in MOL, SDF, or MDL file format)

To edit a library entry, see "Editing a User Library" on page 30.

Managing Libraries

Library Browser can create, manage, and search user libraries. Use these functions to create reference libraries from your own spectra.

Use the Xcalibur data system to create a custom library of MS/MS spectra. The data system includes a subset of the NIST mass spectral library called *nistdemo*. The NIST/EPA/NIH main library contains more than 100,000 compounds whose MS-type spectra were obtained primarily in electron ionization (EI) scan mode. You might want to create a custom library that includes MS/MS spectra or spectra of MS^n analyses.

Contents

- Creating a User Library
- Adding Spectra to a User Library
- Editing a User Library
- Managing the NIST Libraries
- Converting Libraries to Another Format

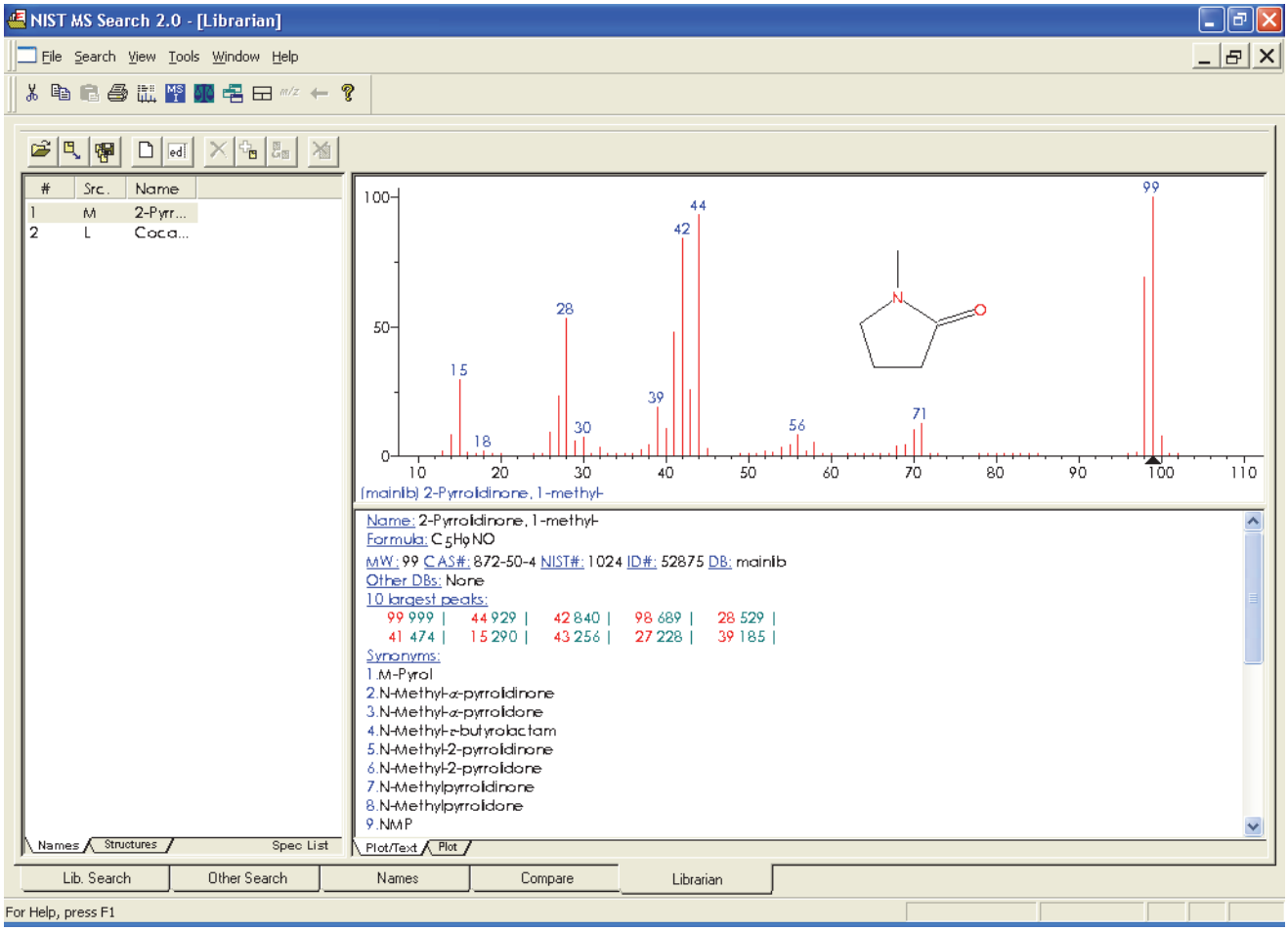
Creating a User Library

You can create a user library in two ways: export a spectrum from Qual Browser or view a spectrum from the Library Browser.

❖ To create a user library from Qual Browser

1. To start a new user library, export a spectrum from Qual Browser. For more information about exporting a spectrum, see "Exporting Spectra from the Xcalibur Data System" on page 22.
2. Choose **Window > Librarian**.
3. In the NIST MS Search 2.0 Librarian window (see Figure 14), select a spectrum.

Figure 14. NIST MS Search 2.0 - Librarian window

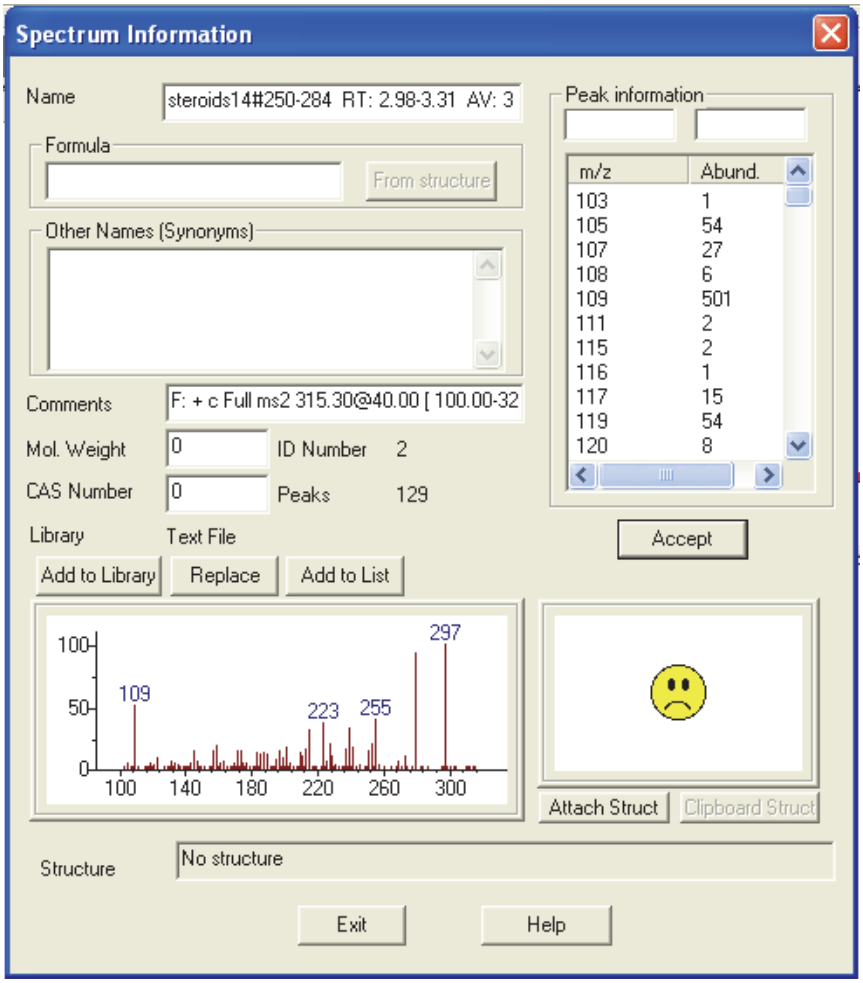


4. Click **Add** in the Librarian window toolbar.

❖ To create a library from the Library Browser window

1. Select a spectrum in the Library Browser window.
2. In the Librarian window, click in the toolbar to display the Spectrum Information Dialog Box (see Figure 15).

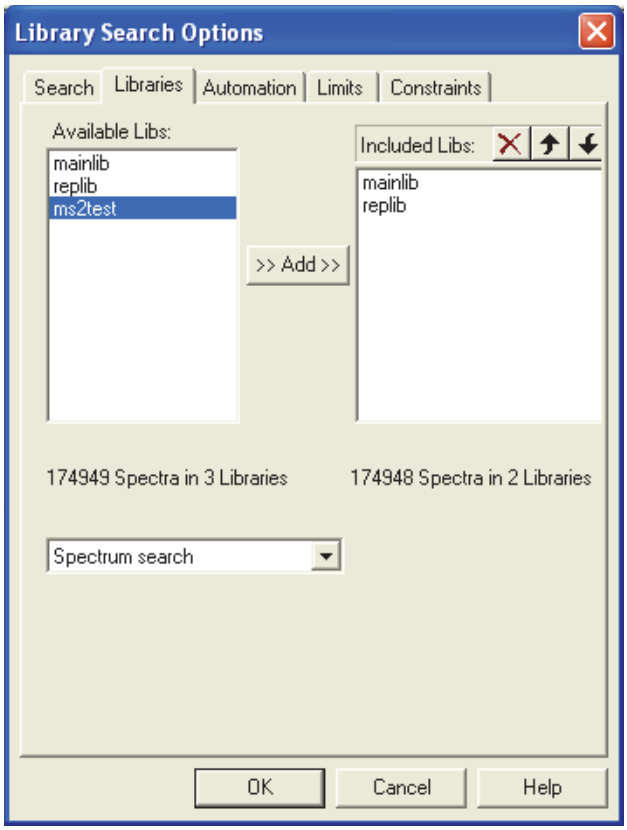
Figure 15. Spectrum Information dialog box



3. Click **Add to Library** to add the spectrum to a new library and name the library. The Choose Library To Copy To dialog box opens.

4. Click the **Libraries** tab to display the Available Libs and the Included Libs list of libraries (see Figure 16).

Figure 16. Library Search Options dialog box

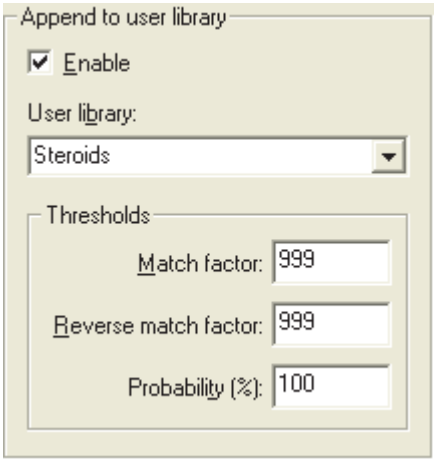


5. Type the name of the new user library.
6. Click **OK** to create the new user library and close the dialog box.

Adding Spectra to a User Library

Use the Append to User Library area, shown in Figure 17, to add processed spectra to a specific user library.

Figure 17. Append to user library area



❖ To set matching criteria to avoid duplicate entries

1. Select the **Enable** check box.
2. Either select a user library from the User Library list or type a new library name. The drop-down list includes all currently active user libraries.

   If you type a new library name, the library is created only if a spectrum fails the matching criteria. Enter the highest possible values in the Thresholds boxes. The failed spectrum is appended to the library.
3. Type threshold values for Match Factor, Reverse Match Factor, and Probability%. To confirm that all spectra are appended to the library, type **999**, **999**, and **100** respectively. See "Submitting a Spectrum to a Library Search" on page 56 for an explanation of these threshold values.

During processing and after any requested enhancement of a relevant chromatogram peak apex scan, the Xcalibur data system submits the spectrum to a library search:

- If the top hit from a library search exceeds (or is equal to) any one of the threshold values, the data system returns the hit list and the spectrum is not appended to the specified library.
- If the top hit fails to reach any of the threshold values, the data system discards the hit list (no search results are reported) and appends the searched spectrum to the specified library. Unless otherwise specified, the library is stored in the NIST\MSSearch folder.

Editing a User Library

To edit a user-library entry that contains an MS/MS spectrum exported from Qual Browser, use the following procedure.

To edit a user library, complete the following tasks detailed in this section:

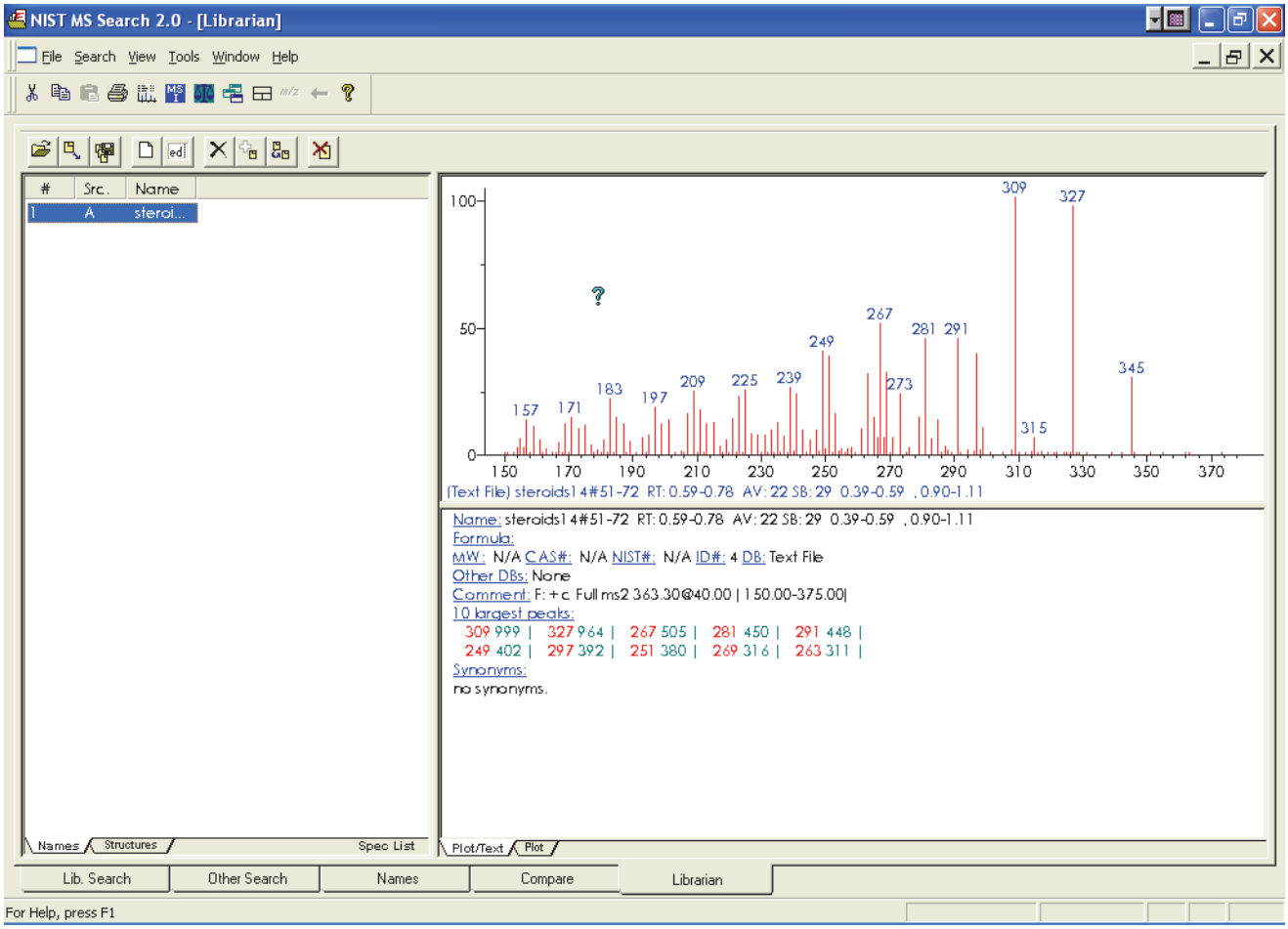
- Editing Spectrum Information
- Attaching a Chemical Structure to a Library Entry
- Adding Additional Compounds to the User Library

Editing Spectrum Information

❖ To edit MS/MS spectrum information in Library Browser

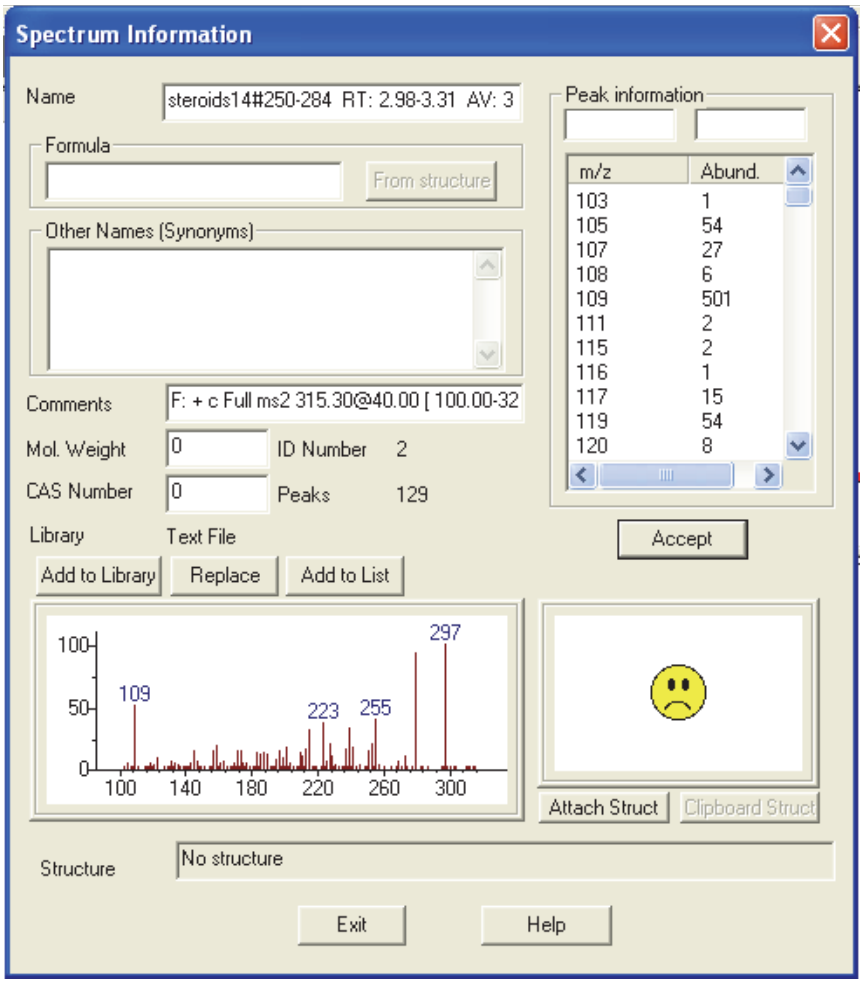
1. Open Library Browser and choose **Window > Librarian**. The Librarian window opens. Because the information for an MS/MS spectrum is stored as a text file, the source of the data is listed as Text File in the Plot/Text pane (see Figure 18).

Figure 18. Librarian window, showing the spectrum information as a text file


NIST MS Search 2.0 - [Librarian]
File Search View Tools Window Help
Src. Name
1 A steroi...
100
50
0
309
327
267
281 291
249
345
273
239
225
209
197
183
171
157
315
150 170 190 210 230 250 270 290 310 330 350 370
(Text File) steroids1 4#51-72 RT: 0.59-0.78 AV: 22 SB: 29 0.39-0.59 , 0.90-1.11
Name: steroids1 4#51-72 RT: 0.59-0.78 AV: 22 SB: 29 0.39-0.59 , 0.90-1.11
Formula:
MW: N/A CAS#: N/A NIST#: N/A ID#: 4 DB: Text File
Other DBs: None
Comment: F: + c Full ms2 363.30@40.00 | 150.00-375.00|
10 largest peaks:
309 999 | 327 964 | 267 505 | 281 450 | 291 448 |
249 402 | 297 392 | 251 380 | 269 316 | 263 311 |
Synonyms:
no synonyms.
Names Structures Spec List
Plot/Text Plot
Lib. Search Other Search Names Compare Librarian
For Help, press F1

2. To display the Spectrum Information Dialog Box box (see Figure 19), click . The dialog box opens, displaying information specific to the spectrum.

Figure 19. Spectrum Information dialog box showing raw spectrum information



3. Give the spectrum a new name:
   a. Click and drag the cursor in the **Name** box to highlight the entire text string.
   b. Change the default text string of the spectrum to a more useful name.

Attaching a Chemical Structure to a Library Entry

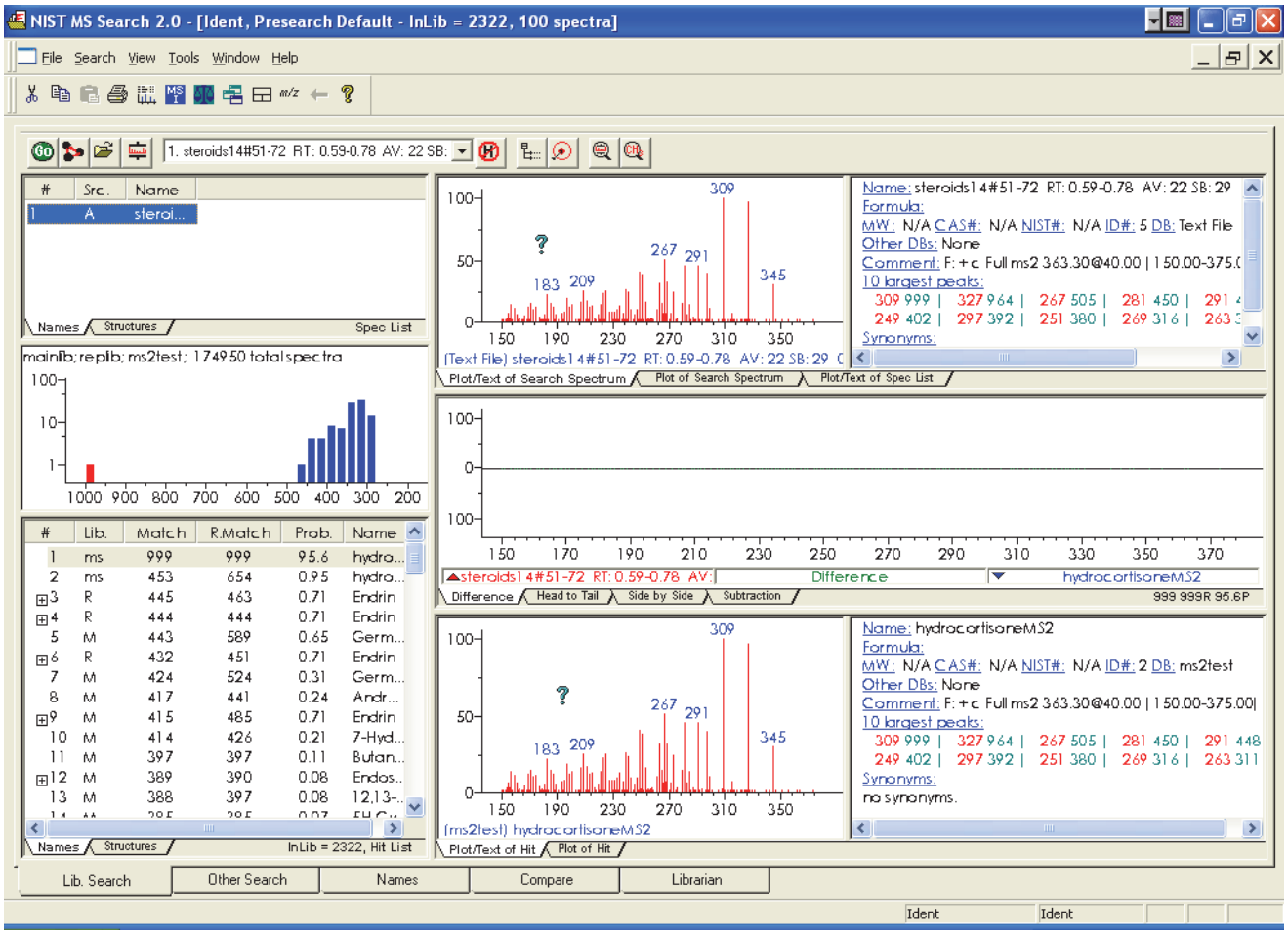
To attach a chemical structure from a list of structures to an entry in a custom library, use the following procedure. Also use the procedure to attach a structure from a program such as ChemDraw™. ChemDraw saves drawings of chemical structures in the .mol file format.

Because you cannot attach a structure to a text file, set the search parameters in Library Browser so that the name of the compound source changes to a name other than Text File in the Librarian window.

❖ To attach a structure to an entry and change the source of the entry

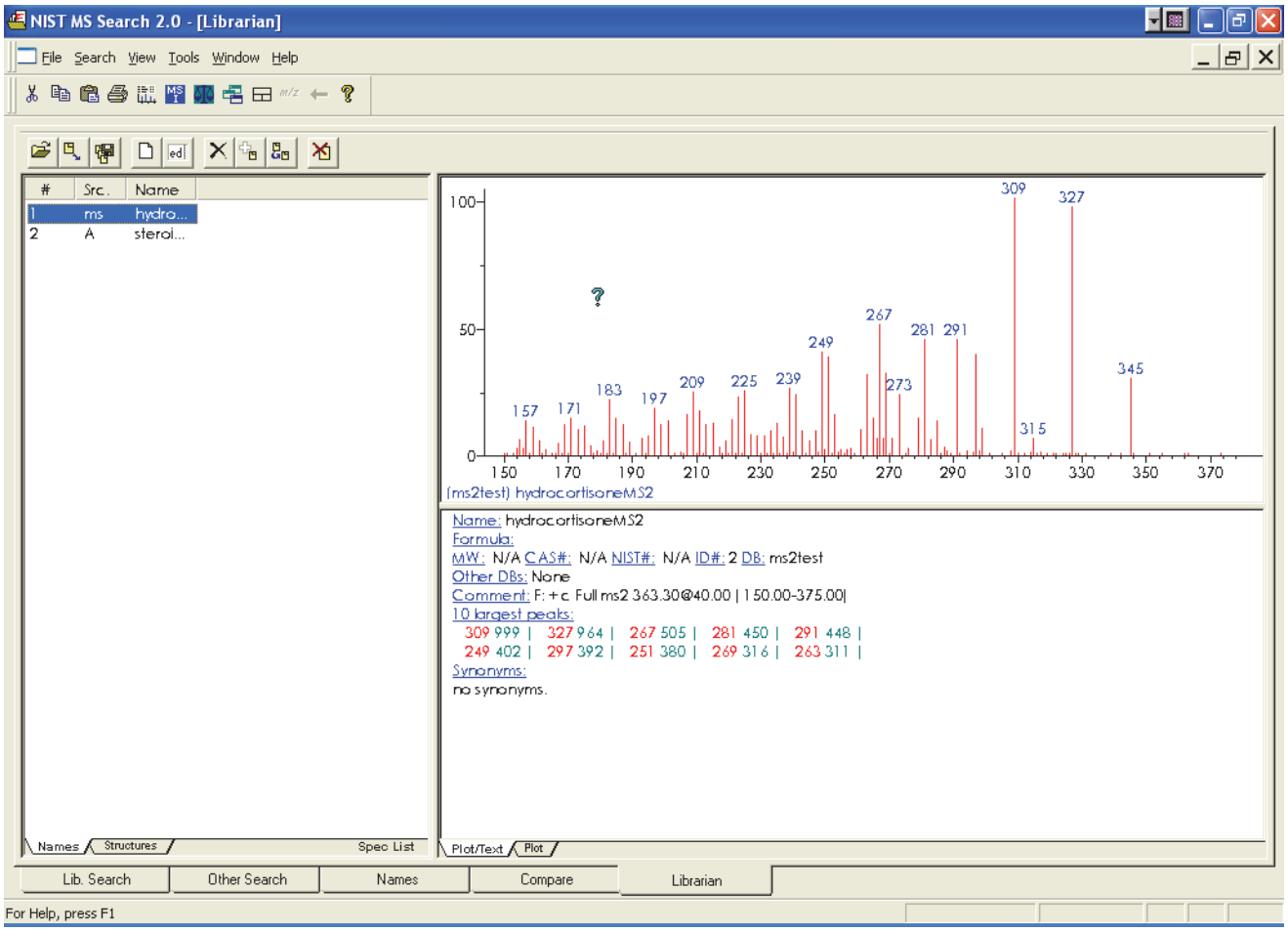
1. Export a spectrum to a library following the instructions in "Exporting Spectra from the Xcalibur Data System" on page 22.
2. From the Lib. Search window, select an entry in the Spec List pane. Right-click this entry and select **Library Search**. Library Browser finds the entry and copies it to the Hit List pane (see Figure 20).

Figure 20. Library Search window, showing the results of searching a library



3. To copy the search result to the Spec List pane:
   a. Select the Hit List entry you just created. Right-click this entry and select **Copy** from the shortcut menu.
   b. To make the Spec List pane active, move the cursor to the Spec List pane and left-click the mouse button.
   c. To paste the entry to the Spec List window, right-click to display the shortcut menu and choose **Paste**.
4. Click the **Librarian** tab. The Librarian window opens (see Figure 21).

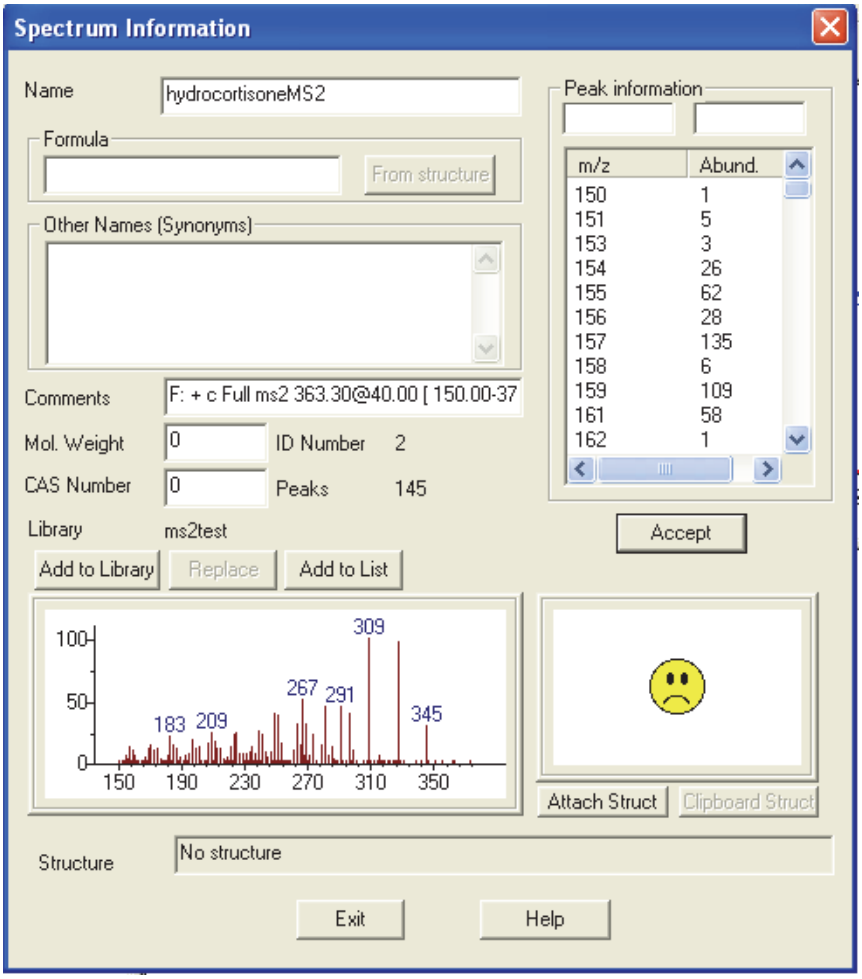
Figure 21. Librarian window



5. To save the structure of the entry from the library to the entry:

   a. In the Librarian window, click in the toolbar. The Spectrum Information dialog box opens (see Figure 22).

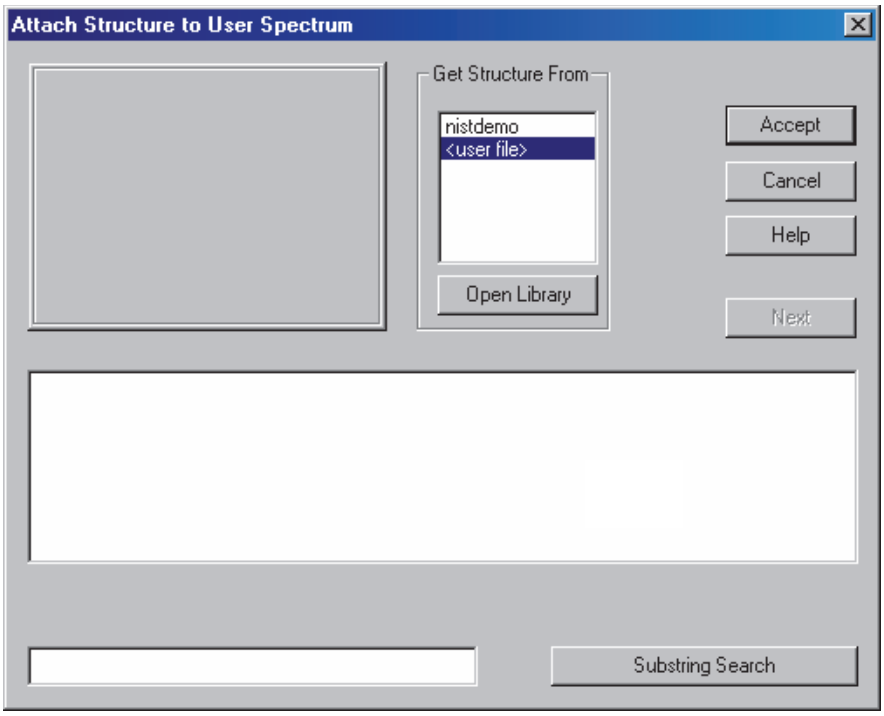
   Figure 22. Spectrum Information dialog box



   b. To search for chemical structure files from other sources, click the **Attach Struct** button. The Open dialog box opens.

c. If the structure you want is not available in the Open dialog box folders, click **Cancel** to search other libraries. The Attach Structure to User Spectrum dialog box opens (see Figure 23).

Figure 23. Attach Structure to User Spectrum dialog box

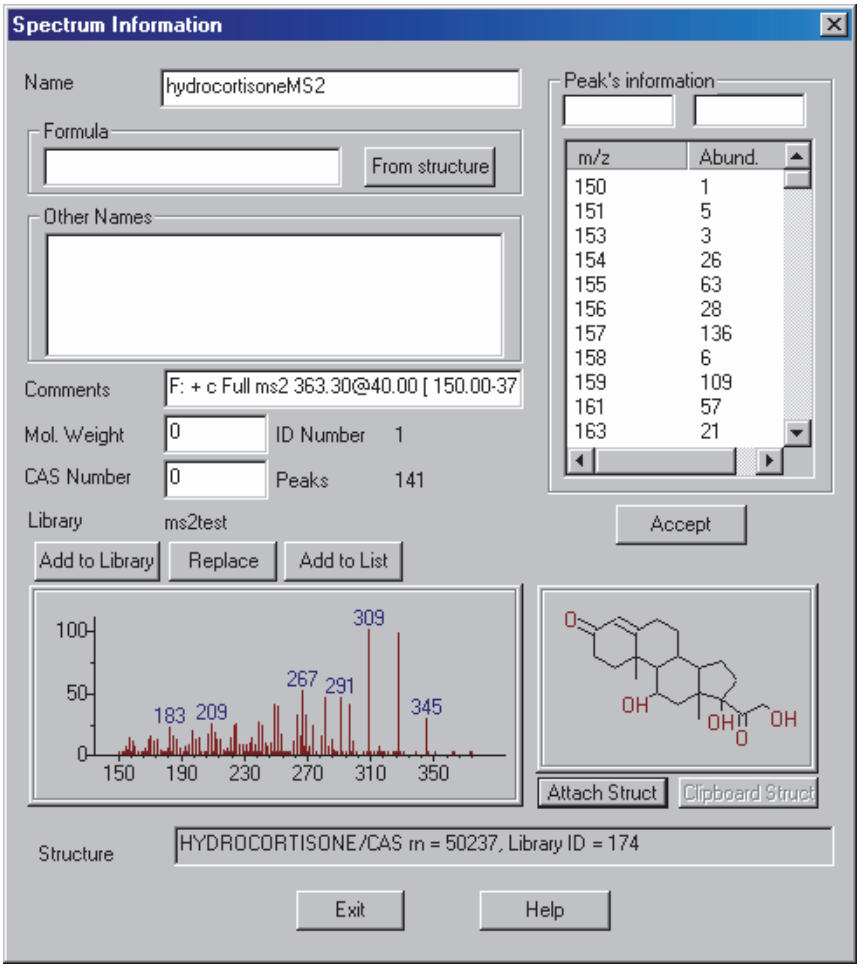


d. Select a library name in the **Get Structure From** area and click **Open Library**.

e. Type the name of the compound to search for in the Substring Search box. Then click **Substring Search**. Library Browser scans the library and finds the MS data and the structure for your entry.

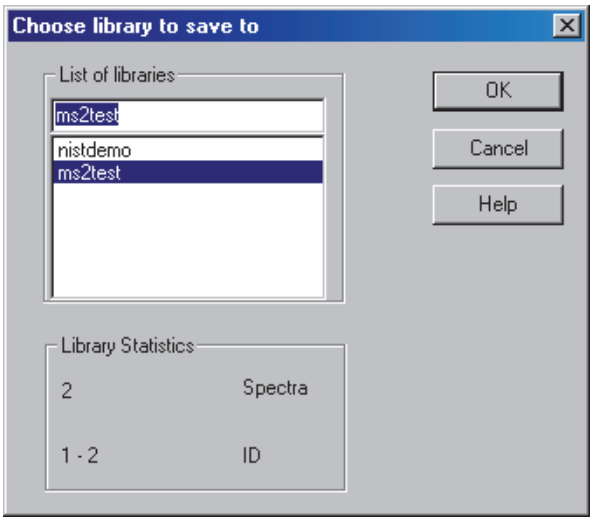
f. To accept the structure and return to the Spectrum Information dialog box (see Figure 24), click **Accept**.

Figure 24. Spectrum Information dialog box, showing the structure to add



g. Click **Add to Library** to display the Choose Library to Save to dialog box (see Figure 25).

Figure 25. Choose library to save to dialog box



h. To save the structure to the library, click **OK**. The application closes the Choose Library to Save to dialog box and opens the Librarian window. The source of the entry appears as the new library name.

6. Highlight the entry in the Spec List. The Text File designation appears in the Plot pane.
7. To delete the entry, click in the toolbar.

   A warning appears.
8. Click **OK** to close the warning dialog box.
9. Click the **Lib. Search** tab to return to Library Browser's Library Search window.
10. Double-click the entry in the Spec List.

    The data system attaches the chemical structure to the library entry.

Adding Additional Compounds to the User Library

To add compounds to a user library, use the Qual Browser window.

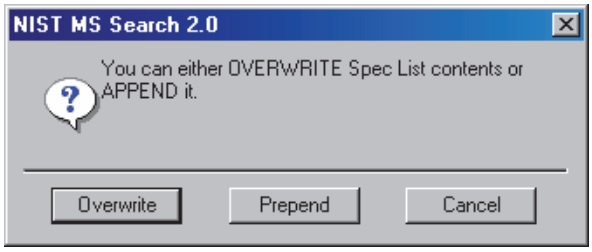
This procedure describes exporting spectra to Library Browser using unenhanced spectra. For more information, see "Working with Background Spectra" on page 18 and the previous section, "Attaching a Chemical Structure to a Library Entry" on page 32. Apply the procedures from these related sections to unenhanced spectra, when possible, before you do the procedure in this section.

❖ To add library entries from Qual Browser to a user library

1. To display the Qual Browser window, click

in the task bar at the bottom of the monitor screen.
2. To display an MS/MS spectrum of a relevant peak:
   a. Click in the Spectrum view (upper right cell) in Qual Browser to make the cell active.
   b. Move the cursor to the Chromatogram view in the lower right cell. Click and hold just to the left of the second chromatographic peak.
   c. To average the scans you select, drag the cursor horizontally across the peak. The Xcalibur data system displays the spectrum in the Spectrum view.
3. Right-click the mass spectrum to display a shortcut menu.
4. To export the spectrum, choose **Library > Export to Library Browser**. The data system displays a message box, as shown in Figure 26.

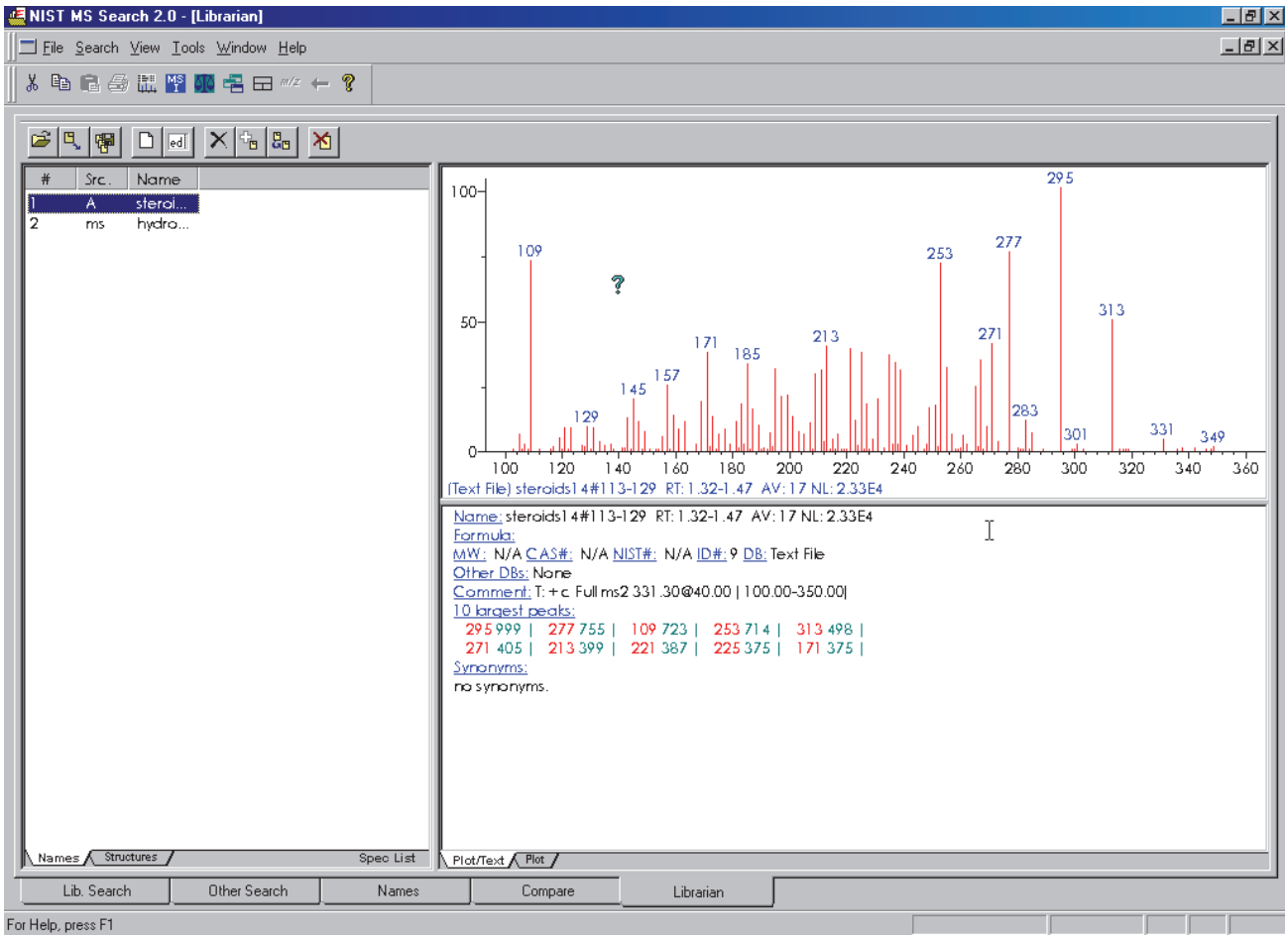
Figure 26. Export Message box



5. To add the entry to the top of the Clipboard window, click **Prepend**.

6. To edit the spectrum information
   a. Display the Librarian window by choosing **Window > Librarian** in Library Browser.
   b. Select the unedited entry in the Spec List pane as shown in Figure 27.

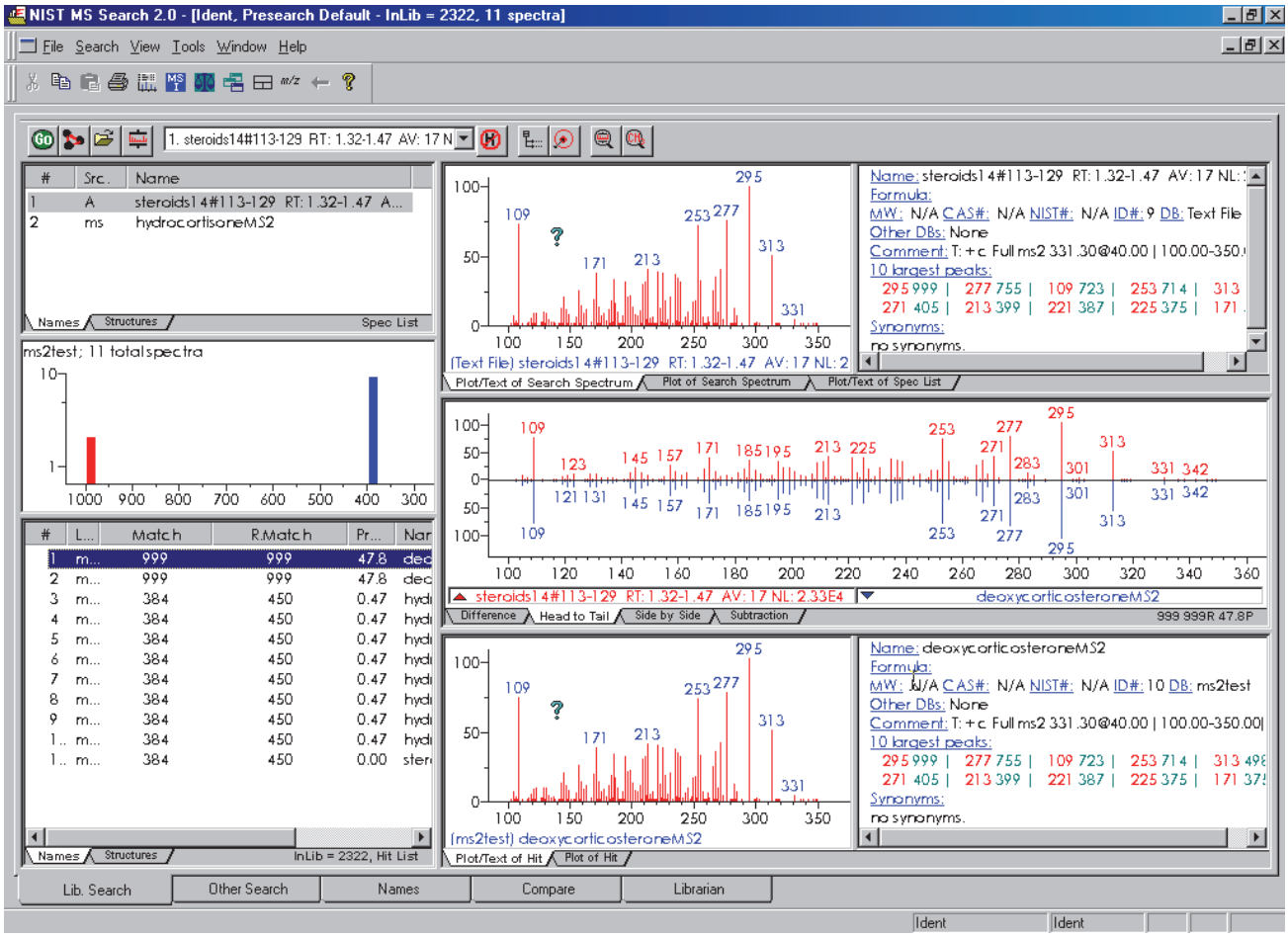
Figure 27. Librarian window, showing a spectrum in a list of entries


NIST MS Search 2.0 - [Librarian]
File Search View Tools Window Help
Src. Name
1 A steroi...
2 ms hydro...
Names Structures Spec List
Plot/Text Plot
Lib. Search Other Search Names Compare Librarian
For Help, press F1
(Text File) steroids14#113-129 RT: 1.32-1.47 AV: 17 NL: 2.33E4
Name: steroids14#113-129 RT: 1.32-1.47 AV: 17 NL: 2.33E4
Formula:
MW: N/A CAS#: N/A NIST#: N/A ID#: 9 DB: Text File
Other DBs: None
Comment: T: + c Full ms2 331.30@40.00 | 100.00-350.00|
10 largest peaks:
295 999 | 277 755 | 109 723 | 253 714 | 313 498 |
271 405 | 213 399 | 221 387 | 225 375 | 171 375 |
Synonyms:
no synonyms.

   c. Click ed. The Spectrum Information dialog box opens.
   d. Select all of the text in the Name box and type a name for the entry.
   e. Click **Add to Library**. The Choose Library to Save to dialog box opens.
   f. To copy the new spectrum entry to the selected library, click **OK**. (The entry Text File in the Librarian window does not change.)

7. To copy and paste the library entry from the Hit List pane to the Spec List pane (see Figure 28):

Figure 28. Library Browser panes, showing the results of a search from the Spec List panel



a. In Library Browser, choose **Window > Lib. Search** to display the Library Search window.

b. Select a file in the Spec List pane. Right-click this entry and choose **Library Search**. If Library Browser finds the entry, the application copies it to the Hit List pane.

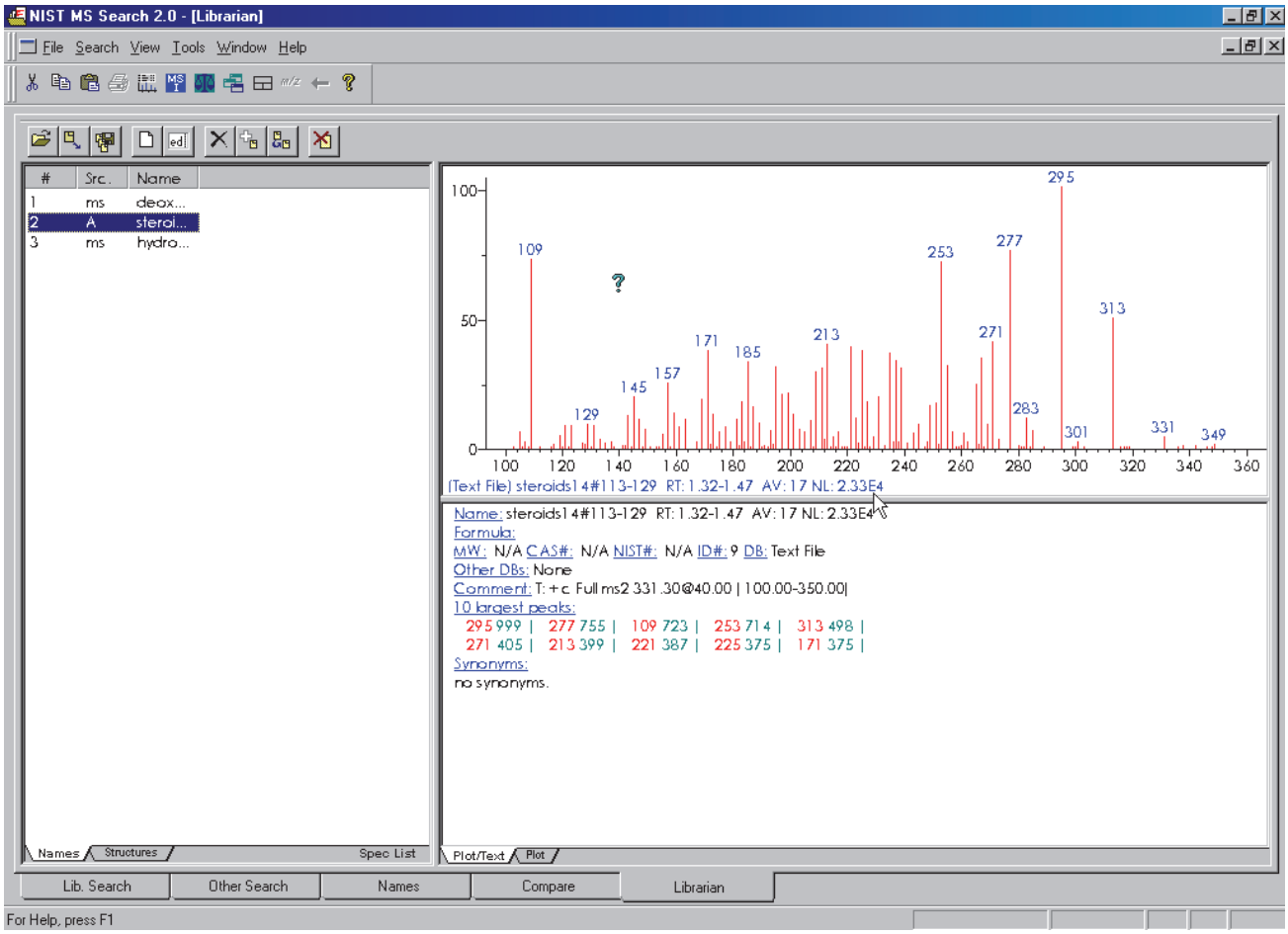
c. Select the search results entry from the Hit List. Right-click this entry and choose **Copy** from the shortcut menu.

d. To make the Spec List pane active, move the cursor to the Spec List pane and left click the mouse button.

e. To paste the entry to the Spec List window, right-click to display the shortcut menu and choose **Paste**.

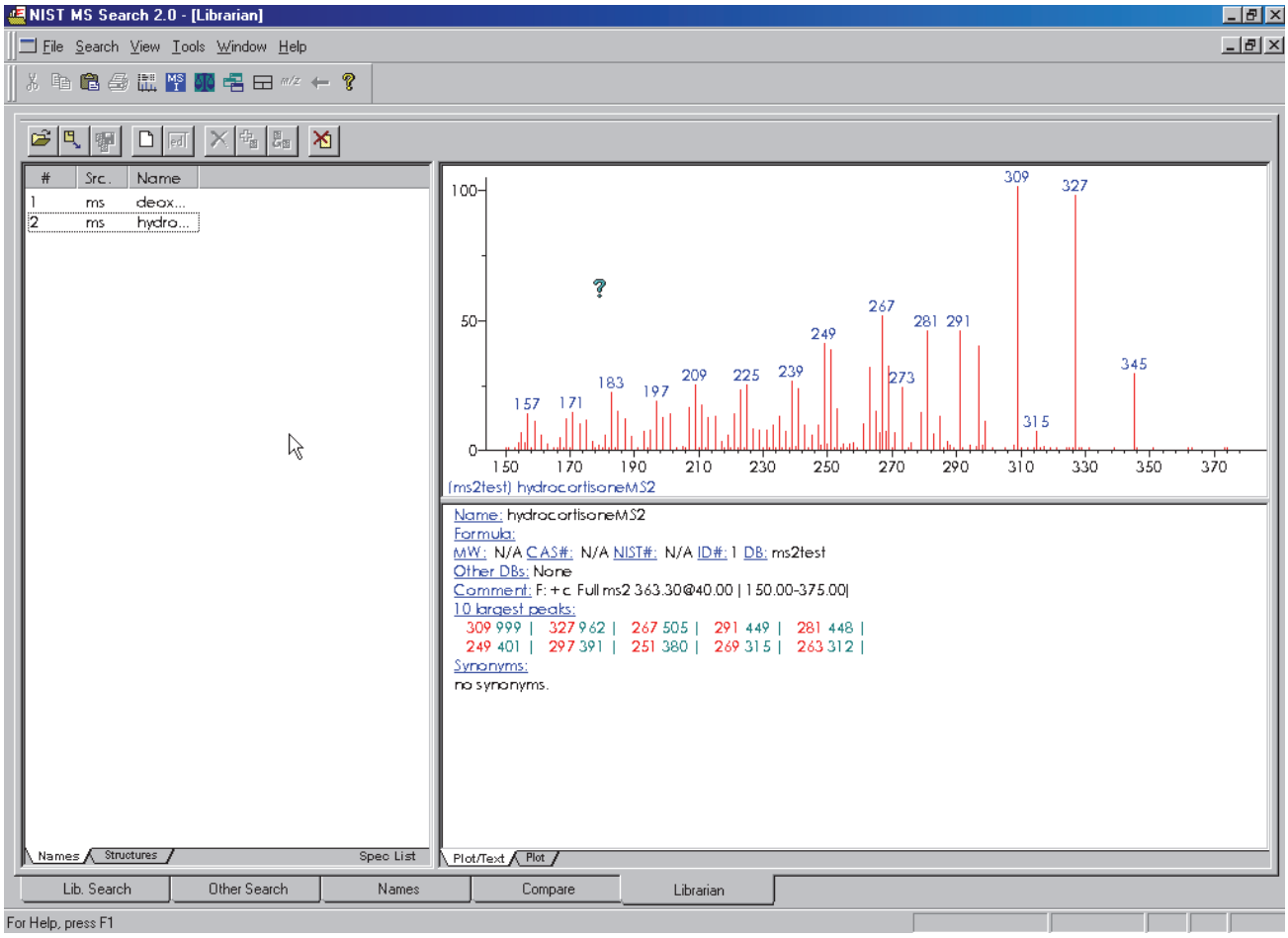
8. Choose **Window > Librarian** to display the Librarian window (see Figure 29).

Figure 29. Librarian window, showing the entry from the source file highlighted


NIST MS Search 2.0 - [Librarian]
File Search View Tools Window Help
Src. Name
1 ms deox...
2 A steroi...
3 ms hydro...
Names Structures Spec List
Lib. Search Other Search Names Compare Librarian
For Help, press F1
Plot/Text Plot
(Text File) steroids14#113-129 RT: 1.32-1.47 AV: 17 NL: 2.33E4
Name: steroids14#113-129 RT: 1.32-1.47 AV: 17 NL: 2.33E4
Formula:
MW: N/A CAS#: N/A NIST#: N/A ID#: 9 DB: Text File
Other DBs: None
Comment: T: + c Full ms2 331.30@40.00 | 100.00-350.00|
10 largest peaks:
295 999 | 277 755 | 109 723 | 253 714 | 313 498 |
271 405 | 213 399 | 221 387 | 225 375 | 171 375 |
Synonyms:
no synonyms.

9. To delete the entry, highlight the entry from the source file and click ✕ in the toolbar (see Figure 30).

Figure 30. Librarian window, showing added entries



10. Close the windows and return to the Xcalibur Home Page:
    a. Choose **File > Exit** to close Library Browser and return to Qual Browser.
    b. Choose **File > Exit** again to close the Qual Browser window and return to the Xcalibur Home Page.

Managing the NIST Libraries

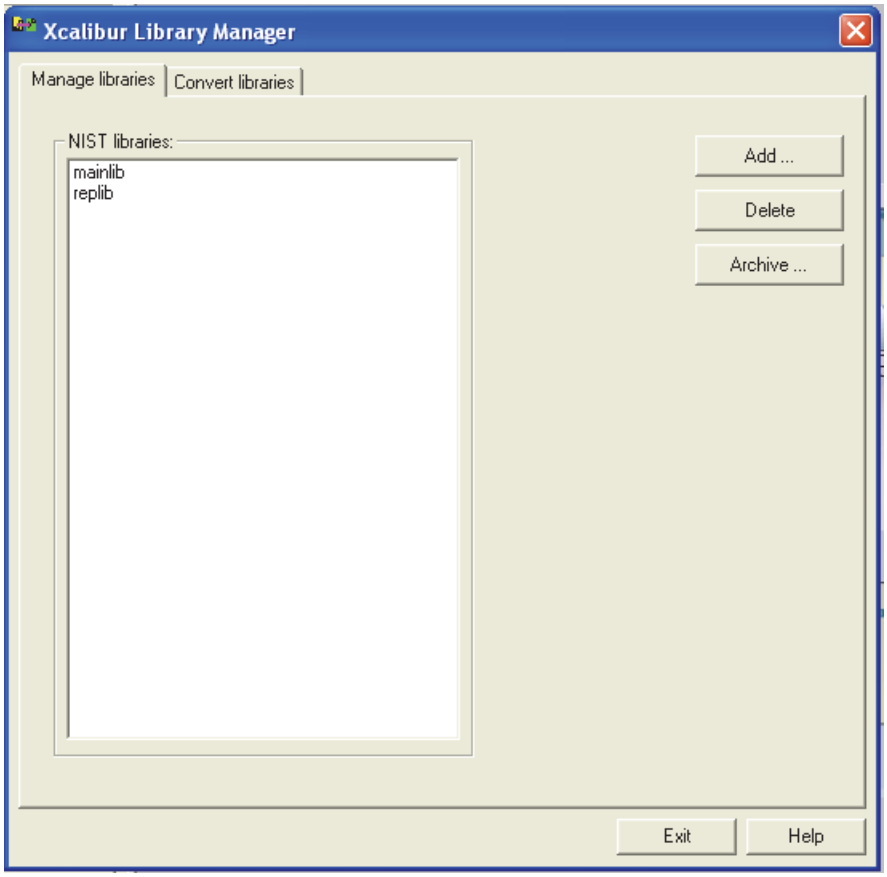
To add, delete, or move a library from the NIST libraries list, use the Manage Libraries page in the Xcalibur Library Manager dialog box. This section shows you how to complete the following tasks:

- Adding a Library
- Deleting a Library
- Copying a Library

❖ To open the Xcalibur Library Manager

1. If the Xcalibur Home Page is not already open on the computer, choose **Start > All Programs > Thermo Xcalibur > Xcalibur**. Verify that the home page is open in the Roadmap view.
2. To open the Library Manager Dialog Box, choose **Tools > Library Manager**. The Library Manager opens on the Manage Libraries page by default (see Figure 31).

Figure 31. Manage Libraries page



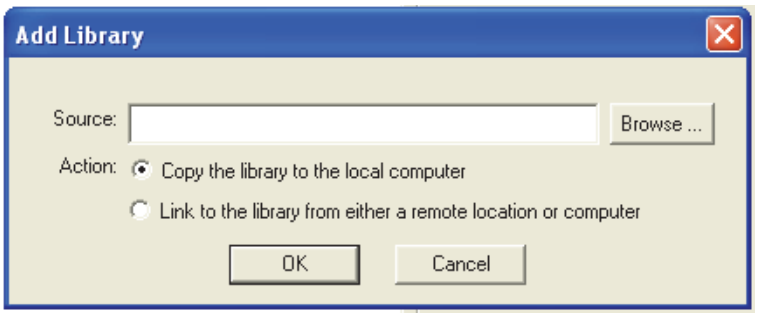
Adding a Library

When you add a library to the NIST libraries list, either copy the library file to the local computer or link to the library at a remote location without copying files.

❖ To add a library

1. In the Library Manager Dialog Box, click **Add**. The Add Library dialog box opens (see Figure 32).

   Figure 32. Add Library dialog box

2. In the Add Library dialog box, type the path for the new library file in the Source field or click **Browse** to bring up the Browse for Folder dialog box and find the desired file.
3. Select one of the two options:
   - Copy the library to the local computer
   - Link to the library from either a remote location or computer

   Note Because libraries can be large, you can often save time by selecting the Link option rather than the Copy option.
4. Click **OK**. The data system adds the desired library to the NIST Libraries list in the Xcalibur Library Manager dialog box.
5. If you have no more tasks to complete with the Library Manager, click **Exit**.

Deleting a Library

❖ To delete a selected library in the NIST Libraries list

1. In the Xcalibur Library Manager dialog box, select a library to delete from the NIST Libraries list.
2. Click **Delete**. The system prompts you to confirm the deletion. To delete the selected library, click **Yes**.
3. If you have no more tasks to complete with the Library Manager, click **Exit**.

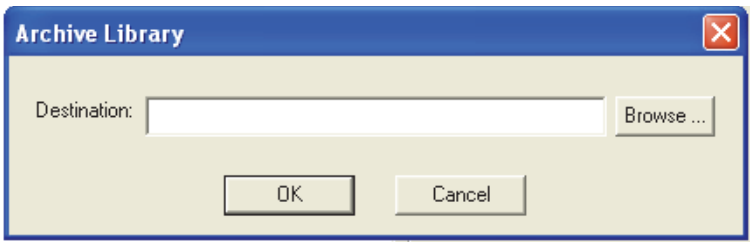
Copying a Library

You can copy a selected library to another directory on the computer or network by using the Archive feature.

❖ To copy a library

1. In the Library Manager Dialog Box, select a library to copy from in the library name in the NIST Libraries list.
2. Click **Archive**. The Archive Library dialog box opens (see Figure 33).

   Figure 33. Archive Library dialog box

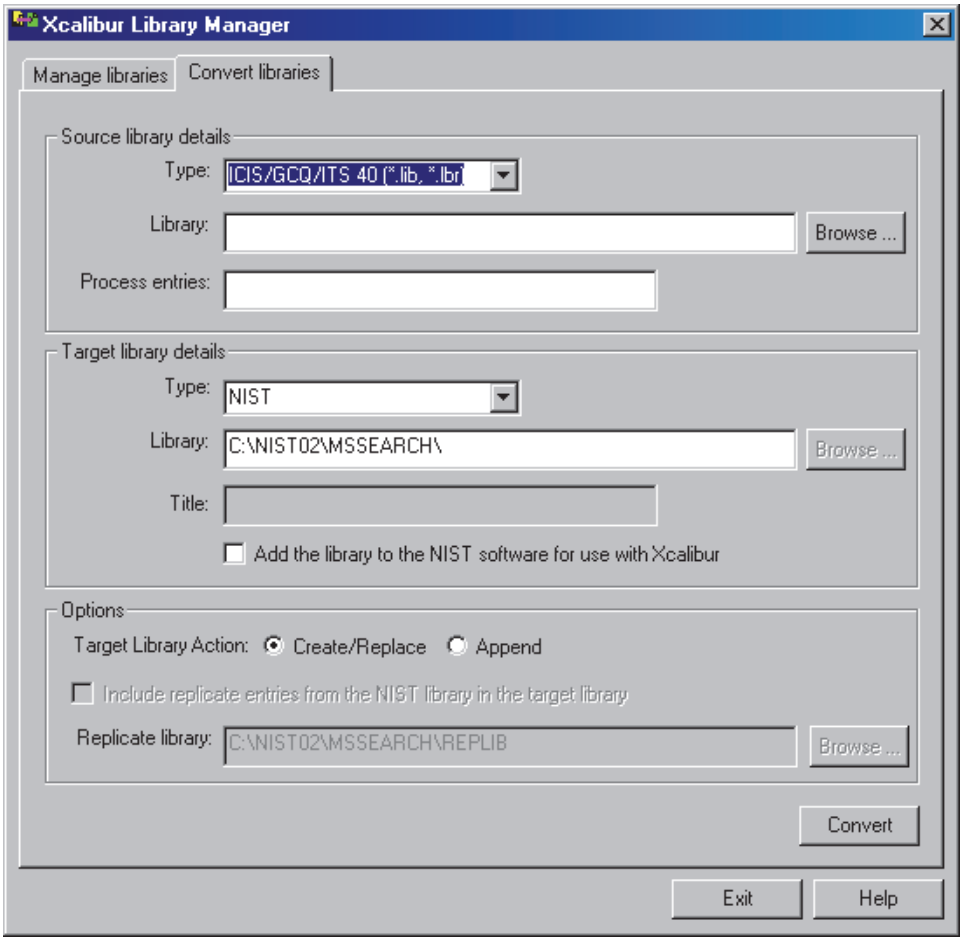
   

3. In the Archive Library dialog box, type the path for the copied library file in the Destination field or click **Browse** to bring up the Browse for Folder dialog box and find the desired location.
4. To copy the desired library to the remote location, click **OK**.
5. If you have no more tasks to complete with the Library Manager, click **Exit**.

Converting Libraries to Another Format

To convert all or any portion of a library to another format, use the Convert Libraries Page in the Library Manager Dialog Box (see Figure 34). Also, use this page to copy a library to another location.

Figure 34. Convert libraries page



❖ To convert a library from one format to another

1. In the Xcalibur Library Manager dialog box, type the following information in the Source Library Details area:
   - Select the type of source library, based on the file extension, from the Type drop-down list.
   - Type the path to the source library in the Library field or click **Browse** to open the Browse for Folder dialog box and find a file.
   - To convert only certain entries from the source library, type the number range of the entries to convert in the Process Entries field. For example, to convert only entries #100 to #200, type **100-200**.

2. Enter the following information in the Target Library Details area:

   - Select the type of target library based on the file extension, from the Type drop-down list.
   - Type the path to the target library in the Library field or click **Browse** to open the Browse for Folder dialog box and find a folder.

     Note When you select NIST as the target library type, the default target library is the library folder for Xcalibur software: C:\NIST02\MSSEARCH\.

     When you select ICIS/GCQ/ITS 40 or MassLab as the target library type, the Title field becomes active.

   - Type the title for the converted library in this field.

3. Make the following choices in the Options area, if desired:

   - Select either the **Create/Replace** option or the **Append** option. Create/Replace is selected by default.

     When you select NIST as the source library type, the Include Replicate Entries from the NIST Library in the Target Library check box becomes active.

   - Click this check box to copy replicate entries.

     When you select the Include Replicate Entries check box, the Replicate Library field is active. The default replicate library is C:\NIST02\MSSEARCH\REPLIB.

   - To use a different replicate library, type the path to the desired library in the Replicate Library field or click **Browse** to open the Browse for Folder dialog box and find a folder.

4. To begin the conversion process, click **Convert**. The Conversion Status box displays sequential chronological (top to bottom) messages such as:

   Started the conversion on SEP 3, 1999 at 10:01, please wait
   Finished the conversion on SEP 3, 1999 at 10:02
   Converted 570 entries

5. If you have no more tasks to complete with the Library Manager, click **Exit** to close the Xcalibur Library Manager dialog box.

Searching Libraries

After you create a custom library of spectra, you can search it or other libraries. Set up libraries to search them automatically or search them manually from Qual Browser or Library Browser.

Contents

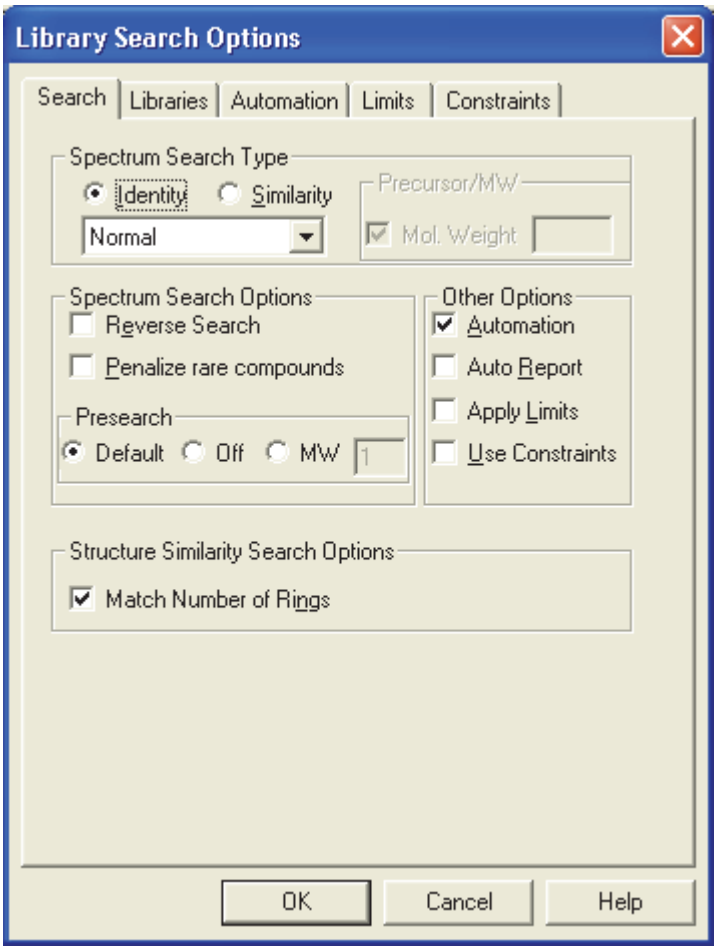
- Customizing a Search
- Setting Library Search Option Parameters
- Submitting a Spectrum to a Library Search
- Limiting a Library Search
- Selecting Libraries to Search
- Setting Up to Search Libraries Automatically
- Processing Raw Files and Printing Reports
- Initiating a Library Search from Qual Browser
- Searching a Library Using Library Browser

Customizing a Search

The Library Browser automatically loads all exported spectra into the Spec List window.

Initiate a library search by double-clicking the appropriate entry. The search uses the settings defined in the Library Search Options Dialog Box (see Figure 35).

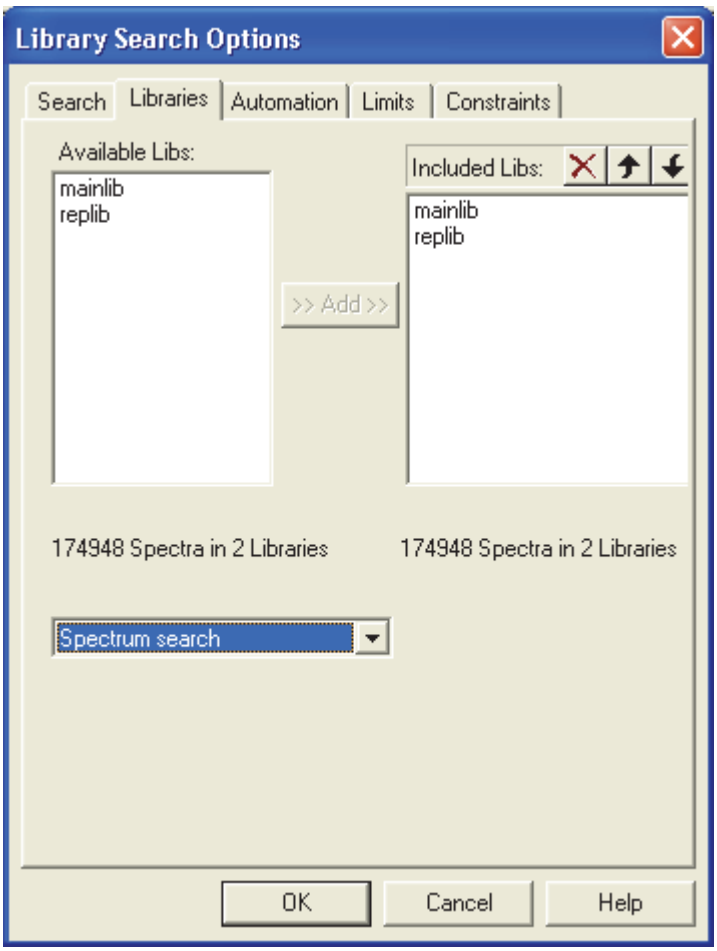
Figure 35. Library Search Options dialog box



Including a User Library in a Search

The default library for a search is the NIST/EPA/NIH main library (*mainlib*), if it is present. Otherwise, the default is a demonstration user library, *nistdemo*. You can add other libraries to the search and change the order of searching on the Libraries page of the Library Search Options dialog box (see Figure 36).

Figure 36. Libraries page of the Library Search Options dialog box



To access this page, click the **Libraries** tab of the Library Search Options dialog box. The Libraries page is divided into two panes:

Available Libs	Lists libraries defined within the Library Browser.
Included Libs	Lists the libraries used by the Library Browser in searches, in the search order.

❖ **To change the search order of included libraries**

Use the up and down arrows.

❖ **To include a library in the search**

1. Select the library name in the Available Libs list.
2. Click **Add**.

❖ **To exclude a library from a search**

1. Select the library name in the Included Libs list.
2. Click the **Delete** button (large red X).

Limiting a Library Search

To examine or modify search constraints, click the **Constraints** tab of the Library Search Options dialog box.

Constraints are divided into six categories:

- Molecular Weight
- Name Fragment
- Elements Value
- Elements Present
- Peaks
- Other Databases

For details about limiting a library search, see "Library Search Constraints Page (Library View)" on page 115.

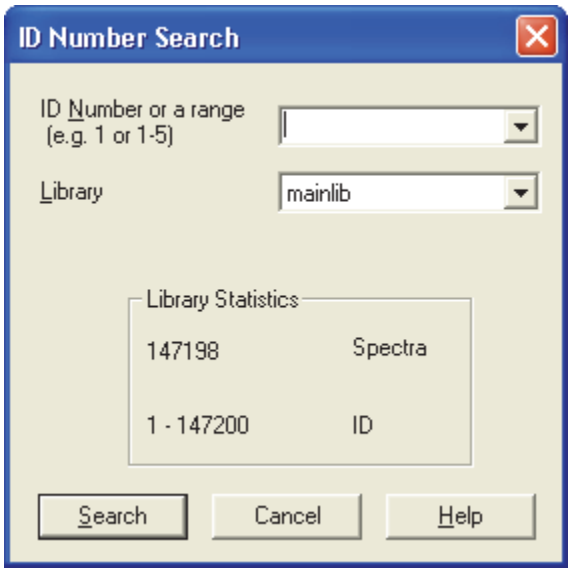
Searching a User Library Entry by ID Number

To search entries in existing libraries, search for a library spectrum by Formula, ID Number, Molecular Weight, Any Peaks, CAS Number, Sequential Method, NIST Number, or Name. Use ID Search if other information is not available or to find a spectrum exported from a processing method.

❖ To search a library by ID Number

1. To open the ID Number Search dialog box (see Figure 37), choose **Search > ID Number** from any Library window.

   Figure 37. ID Number Search dialog box

   The Library Statistics area shows the number of available spectra.

2. To consider all spectra, specify a range in the ID Number box that is equal to or larger than the ID range shown in the Library Statistics area.
3. Select the appropriate user library in the Library drop down list.
4. Click **Search**. The Xcalibur data system writes all entries within the specified range to the Lib. Search area.
5. To copy a spectrum to be edited into the Spec List from the Library Search window, select the spectrum name in the Hit List and use the mouse to drag the selection to the Spec List window.

Setting Library Search Option Parameters

Use the Library Search Options page (see Figure 38) to specify how the library search is carried out.

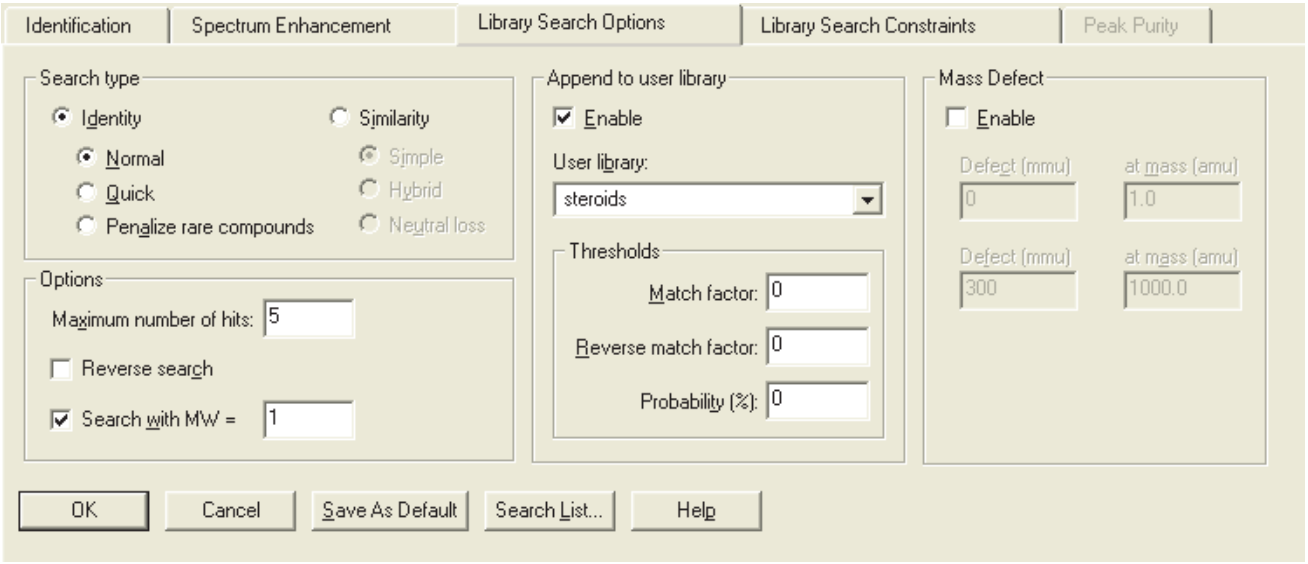
❖ To set Library Search Option parameters

1. Open the Search Parameters Page of the Search Properties dialog box:

   From the Qual Browser window, choose **Actions > Library > Options** or right-click within a Spectrum view and select **Library > Options** from the popup context menu.

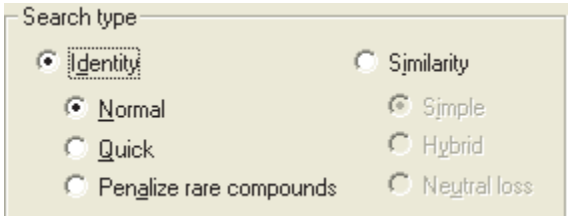
   Click the **Library Search Options** tab.

Figure 38. Library Search Options page from Qual View



2. To submit processed spectra to an identity search, select an **Identity** option in the Search Type area.

   Figure 39. Search type area default settings



3. Choose one of the three Identity search types:

   - Select the **Normal** option to use a normal identity search.
   - Select the **Quick** option to use a quick identity search.
   - Select the **Penalize Rare Compounds** option if you want a modified normal identity search.

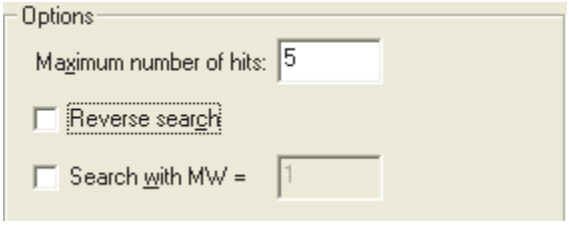
4. To submit processed spectra to a similarity search, select the **Similarity** option. Then choose one of the three Similarity search types:

   - Select the **Simple** option to use a Simple Similarity search.
   - Select the **Hybrid** option to use a Hybrid Similarity search.
   - Select the **Neutral Loss** option if you want a Neutral Loss Similarity search.

   The difference between the two search types is primarily in the weightings of the spectrum as a function of mass.

5. To limit the number of search results to be returned by a library search and reported in the result file, type a number in the Maximum Number of Hits box.

   Figure 40. Options area default settings



6. If you know the molecular weight of your target analyte and want to restrict the search to library compounds of the same molecular weight, select the **Search with MW =** check box and type the molecular weight in the associated box.

   Do not use the Search with MW= option when you have already clicked the Molecular Weight option on the Library Search Constraints page.

7. To include mass defect values for library searches, select the **Enable** check box in the Mass Defect area.

8. Select a sorting method for hits in the result file in the Options area. The Options area shown in Figure 40 contains three ways to customize the library search. The Reverse Search and Search with MW = options are normally not active.

   - To have the Xcalibur data system sort hits by Reverse Match Factor, select the **Reverse Search** check box.
   - To have the Xcalibur data system sort hits by the Forward Match Factor, clear the **Reverse Search** check box.

9. To add new spectra to a user library:

   a. In the Append to User Library area check box, select Enable.

   b. From the User Library list, select the target user library.

   c. Type a threshold value for Match Factor in the Match Factor box.

   d. Type a threshold value for Reverse Match Factor in the Reverse Match Factor box.

   e. Type a threshold value for Probability % in the Probability % box.

10. To save the new settings and close the dialog box, click **OK**.

Submitting a Spectrum to a Library Search

❖ **To submit a spectrum in a Qual Browser spectrum view to a library search**

1. To open a Chromatogram view:
   a. Click in the cell where you want to open the Chromatogram view.

      The data system changes the icon to to indicate that it is the active cell.

   b. Choose **View > Chromatogram** or click on the toolbar.
2. To open a Spectrum view:
   a. Click in the cell where you want to open the Spectrum view.

      The application changes the icon to to indicate that it is the active cell.

   b. Choose **View > Spectrum** or click on the toolbar.
3. To display or enhance a spectrum, choose from these options:
   - With the spectrum cell pinned, click the chromatogram at the point of interest (a peak apex, for example).
   - To view a spectrum averaged across a peak, drag the cursor through the chromatogram peak of interest. For more information, refer to "Selecting a One-Dimensional Range on a Plot" in Chapter 3 of the *Xcalibur Qualitative Analysis User Guide*.
   - Enhance the spectrum, if necessary, by using background subtraction. For more information on this step, see "Working with Background Spectra" on page 18.
4. Select the search libraries and other search options. For more information, see "Setting Library Search Option Parameters" on page 54.
5. To start the library search, choose one of these options:
   - Choose **Actions > Library > Search**
   - Click on the toolbar
   - Right-click the Spectrum View and select **Library > Search** from the context menu

   Qual Browser displays the results of the library search in a Library Search Results window. For more information about this window, see "Library Search Results Window" on page 123.

Limiting a Library Search

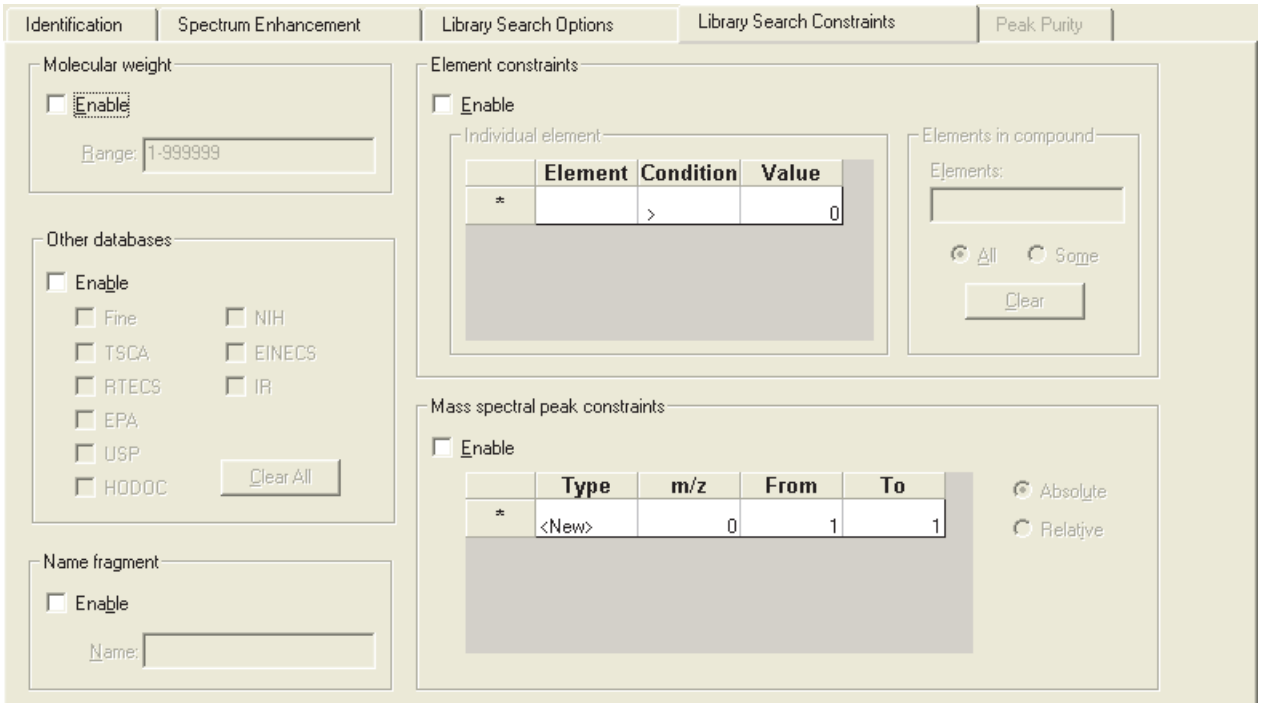
For processing efficiency, constrain a library search using some of the options on the Library Search Constraints page (these are all normally not active). For example, you can exclude certain high intensity ions that appear in many compounds or that are present in the spectrum background. You can target a search to a particular range of molecular weights or to compounds containing certain elements.

Using Library Search Constraints requires specific knowledge about the target compounds in the chromatogram. This knowledge is not always possible in automated processing.

The Library Search Constraints page (see Figure 41) contains five groups of options to constrain the library search. To display the Library Search Constraints page, from the Qual view of the Processing Setup window, select the **Library Search Constraints** tab. See the following sections to set these constraints.

- Applying a Molecular Weight Constraint
- Applying the Other Databases Constraint
- Applying a Name Fragment Constraint
- Applying Element Constraints
- Applying Mass Spectral Peak Constraint

Figure 41. Library Search Constraints page from Qual View



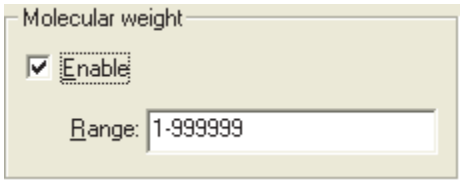
Set parameters and save your settings by clicking **OK**. To save your settings as a default for future searches, click **Save as Default**.

Applying a Molecular Weight Constraint

❖ **To limit the library search to compounds with a specific molecular weight or molecular weight range**

1. Select the **Enable** check box in the Molecular Weight area (see Figure 42).

   Figure 42. Molecular weight area

2. To type a molecular weight or molecular weight range, use the Range box. To specify a range, use the format *low mass - high mass*. The valid range is 1 to 999999. All search results must satisfy the specified molecular weight range.

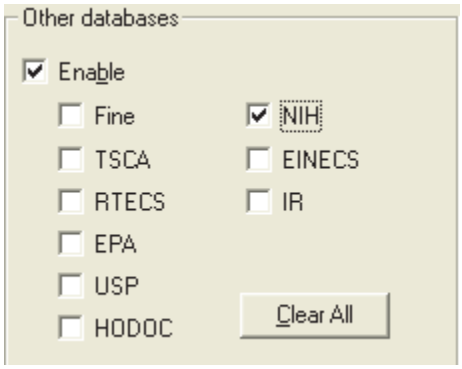
Note This constraint is not available if you have already clicked the Search with MW= option on the Library Search Options page.

Applying the Other Databases Constraint

❖ **To limit the library search to entries in the NIST library that are also featured in other databases**

1. Select the **Enable** check box in the Other Databases area (see Figure 43). NIST library entries contain references to other commercial databases if they contain information about the compound.

   Figure 43. Other databases area

2. Select one or more databases from the available list. To use a database constraint, select its check box. If you do not want to use a database constraint, make sure its check box is clear.

Fine	Commercially Available Fine Chemical Index
TSCA	Toxic Substances Control Act Inventory
RTECS	Registry of Toxic Effects of Chemical Substances
EPA	EPA Environmental Monitoring Methods Index
USP	US Pharmacopoeia/U.S.A.N.
HODOC	CRC Handbook of Data of Organic Compounds
NIH	NIH-NCI Inventory File
EINECS	European Index of Commercial Chemical Substances
IR	NIST/EPA Gas Phase IR Database

The data system only reports search results if they feature in one or more, but not necessarily all, of the selected databases.

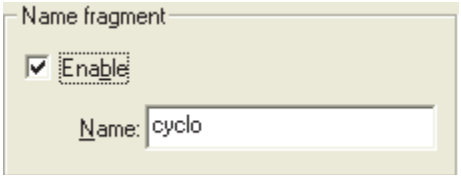
Applying a Name Fragment Constraint

❖ **To limit the search to compounds with a specific name or name fragment**

1. Select the **Enable** check box in the Name Fragment area.

   The Name box accepts a text string (up to 39 characters) to represent a fragment of a compound name; for example, “cyclo”. The library search filters search results and only returns those containing the specified text in their names. The entry is not case sensitive; for example “CYCLO” returns compounds containing the fragments “cyclo”, “Cyclo”, “CYCLO” and any other case permutations.

   Figure 44. Name fragment area



2. Type a name fragment in the Name box.

Applying Element Constraints

To constrain the library search to compounds with specific element profiles, select the **Enable** check box in the Element Constraints area. There are two methods:

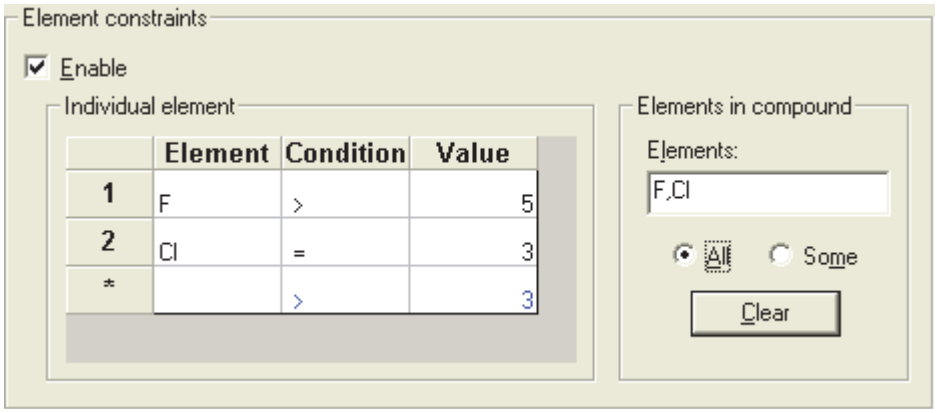
- Individual Element
- Elements in Compound

❖ To use the Individual Elements constraints

1. Click the **Element** box. Type the required element abbreviation.

   Use this area to set specific criteria about the elements required in a library search result (hit). For example, the entries shown in Figure 45 would only return search results for compounds that contain more than five fluorine atoms and exactly three chlorine atoms.

   Figure 45. Element constraints area

   You do not need to provide a complete elemental profile. The library search returns compounds if they satisfy all the specified criteria regardless of any other elements present. Use this option to specify which elements you do **not** want to be in a library hit. For example, C = 0 confirms that no search results contain carbon.

   When a contradiction occurs, for example, C < 2, and C > 4, the data system displays an error dialog box. Correct the contradiction to proceed.

2. In the same row, click the **Condition** list. Click the arrow and select from the three available conditions: < (less than), > (greater than), or = (equal to).

3. In the same row, click the **Value** box. Type the required number of elements for the element constraint condition.

4. Repeat Steps 1 - 3 on the next available row to add further elements to the table.

❖ To use the Elements in Compound constraints

1. Select the **Elements** box and type the IUPAC approved abbreviation for each element (see Figure 45) that must be present in returned search results. Separate each element in the list (of up to 30 characters) by the character specified as the list separator character. Refer to "Changing the List Separator Character" in Chapter 2 in the *Acquisition and Processing User Guide* for more information.
2. Select the **All** option to have the returned search results contain all, and only, the listed elements. For example "C, H, O" would return HCHO but not CO_2, CH_4, or CH_2Cl_2.
3. Select the **Some** option to have the returned search results contain at least one of the specified elements and no elements other than those listed. For example "C, H, O" would return CO_2, CH_4, and HCHO but not CH_2Cl_2 (Cl not allowed).

   If you leave the box blank, the data system does not apply the Elements in compound constraint function. If you type an invalid element, the data system reports an error when the edit field loses focus.

If there are no contradictions, you can use the two types of elemental constraints together. For example, if the Individual Element area contains "C=0" or "C<1" in and the Elements In Compound box contains "C" when the All option has been selected, the data system displays an error dialog box. Correct the contradiction to proceed.

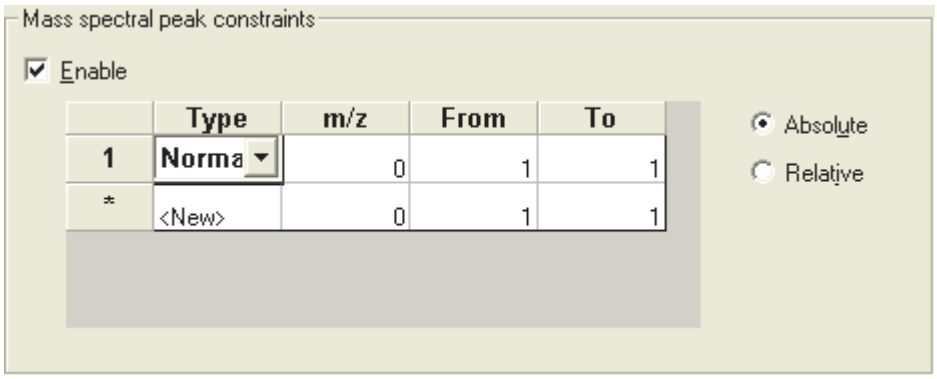
Applying Mass Spectral Peak Constraint

The Mass spectral peak constraint feature builds a profile of ions and their abundances to be matched against library entries during the search.

❖ To apply mass spectral peak constraints

Select **Enable** in the Mass Spectral Peak Constraints area. The search algorithm only returns search results matching the specified constraints.

Figure 46. Example of a relative mass spectral peak constraint



❖ To specify how the data system applies the From and To parameters in the Mass spectral peak constraints table

1. To evaluate all table entries as a percentage of the base (largest) ion in the spectrum, select the **Absolute** option.
2. To treat the first entry as an absolute Normal or Loss type, select the **Relative** option. The software considers subsequent entries in the table relative to the first.
3. In the Mass Spectral Peak Constraints table, click the first available **Type** list. Click the arrow and select from the four available conditions: **Normal**, **Loss**, **Rank** or **Maxmass**.
4. In the same row, select the ***m/z*** box. In a Normal, Rank or Maxmass type constraint, use this box to type the *m/z* value of the mass spectral peak to be constrained. In a Loss type constraint, use this box to type the value of a neutral loss.
5. In the same row, select the **From** box. In a Normal, Loss or Maxmass type constraint, use this box to type the minimum abundance of the constrained mass spectral peak. In a Rank type constraint, use this box to type the lowest position of the ion in an intensity ordered list of spectral peaks.
6. In the same row, select the **To** box. In a Normal, Loss or Maxmass type constraint, use this box to type the maximum abundance of the constrained mass spectral peak. In a Rank type constraint, use this box to type the highest position of the ion in an intensity ordered list of spectral peaks.
7. Repeat steps 3-6 on the next available row to add further peaks to the Mass Spectral Peak Constraints table.

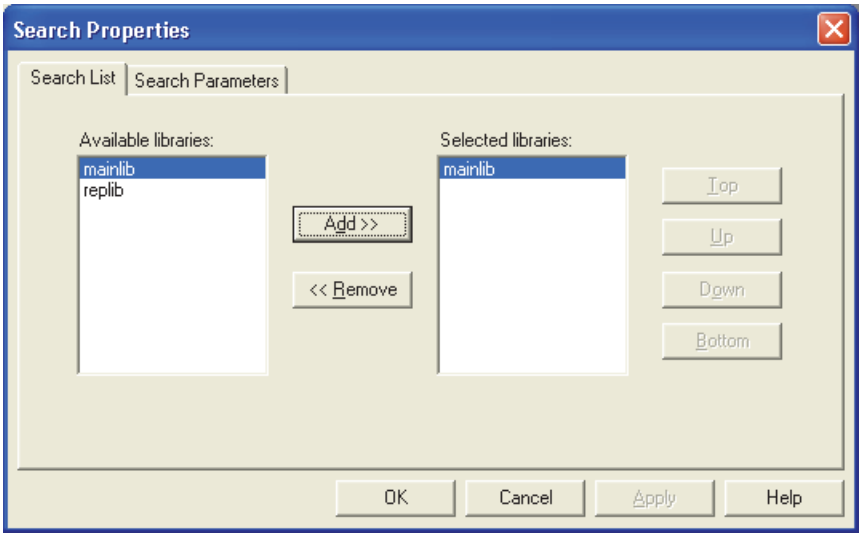
   If you specify the same number in both fields, the designated ion must have that rank in the retrieved spectrum.

> **Note** If you switch between Absolute and Relative modes, the Xcalibur data system prompts you with a warning dialog box before clearing all rows in the grid.

Selecting Libraries to Search

To select a library to search, click Search List... on the Library Search Options page (see Figure 38 on page 54). The Search List page of the Search Properties dialog box opens (see Figure 47). This dialog box lists the names and search order of libraries to be used in library search processing. The list on the left of the dialog box shows the available libraries. The list on the right of the dialog box shows the selected libraries in their search order.

Figure 47. Search List view



The Xcalibur data system generates the Available Libraries list dynamically. Each time you open the Search Properties dialog box, the current list of libraries available on the system at that time appears. This current list might display libraries that do not exist on the system—they might have been selected on another system or deleted or renamed since the method was created.

When you click **OK** in the Search List view, all libraries in the Selected Libraries list are checked. If any of them do not exist, a warning dialog box opens.

❖ To include a library in the search list

1. To open the Search Properties dialog box, choose from these options:
   - From the Qual Browser window, choose **Actions > Library > Options** and click the **Search List** tab.
   - Right-click within a Spectrum view, select **Library > Options** from the shortcut context menu, and click the **Search List** tab.
   - Click **Search List** Search List... on the Library Search Options page (see Figure 38 on page 54).
2. Select the library name in the Available Libraries list.
3. Click **Add** to add the library to the Selected Libraries list in the final position.

❖ **To change the search order of selected libraries**

Select the library name in the Selected Libraries list:

- Click **Top** to move the library to the top of the list.
- Click **Up** to move the library up one position.
- Click **Down** to move the library down one position.
- Click **Bottom** to move the library to the last position.

❖ **To exclude a library from the search list**

1. Select the library name in the Selected Libraries list.
2. Click **Remove** to transfer the library to the Available Libraries list.
3. Click **OK** to save the new settings and close the dialog box.

Setting Up to Search Libraries Automatically

❖ **To set up method files in the data system that search libraries automatically**

1. Use the Xcalibur Processing Setup window to create a processing method file (.pmd).
2. Use the Sequence Setup window to process data files in a sequence list (.sld) with the processing method that you created. For more information about setting up sequences and processes, refer to the *Processes and Sequences User Guide*.

To set up for automatic searching, complete the following procedures:

- Specifying Search Parameters in the Qual View
- Specifying Report Options for Library Searches
- Specifying Raw Data Files in Sequence Setup

Specifying Search Parameters in the Qual View

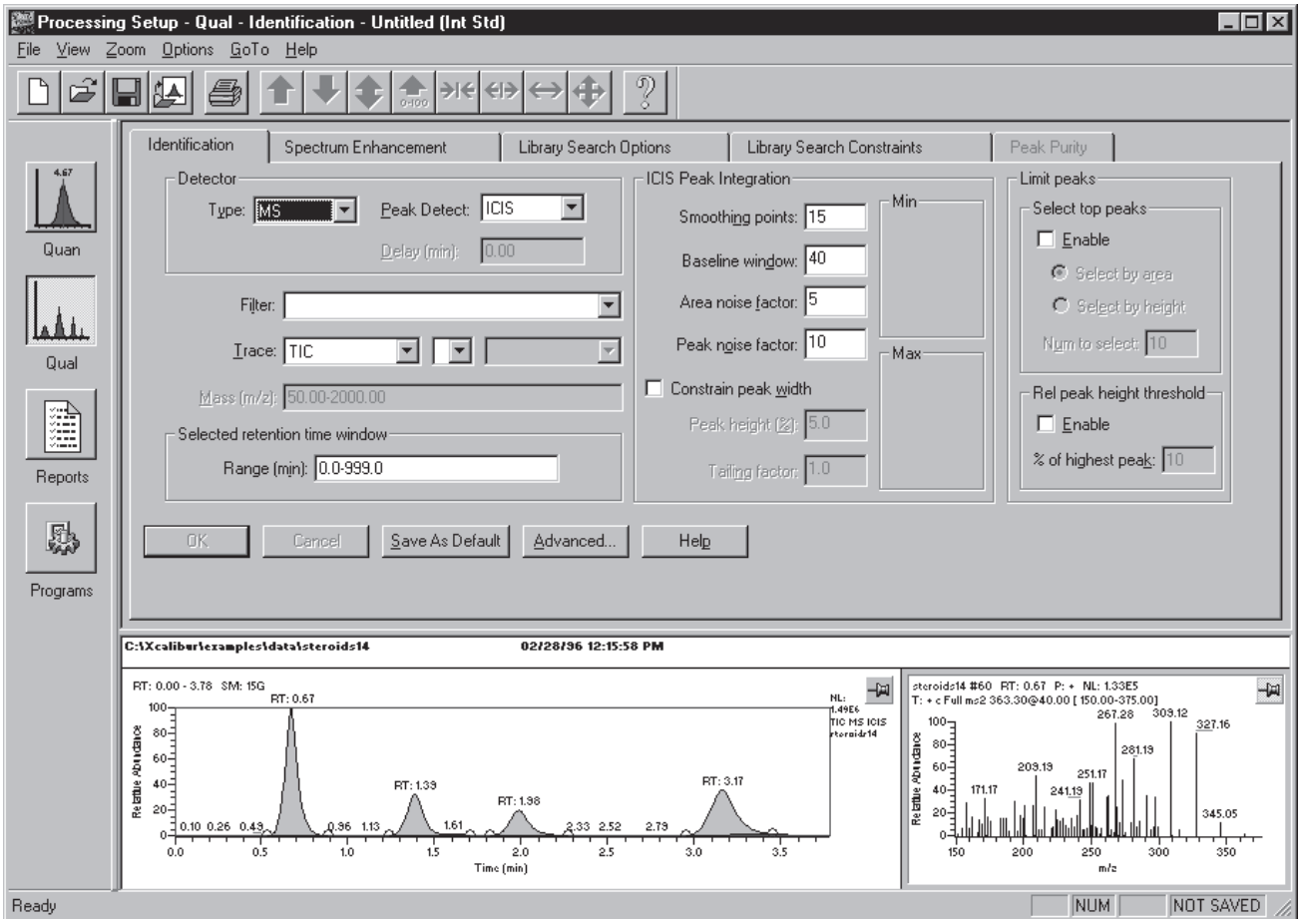
To search libraries automatically, set up the Qual view in the Processing Setup window. For this example, use steroids data.

Note Using the Library Search Constraints page requires specific knowledge about the target compounds in the chromatogram. It is not always possible to use this knowledge to refine automated processing.

❖ To specify parameters for a qualitative library search in the Qual view

1. To open the Processing Setup window, from the Xcalibur Home Page, click .
2. Open a raw data file in the Qual view:
   a. To display the Qual view, click . on the view bar.
   b. To display the Open Raw File dialog box, choose **File > Open Raw File**.
   c. To display the raw data, select a raw file and click **Open** (see Figure 48).

Figure 48. Processing Setup window



3. Select a detector type on the Identification page.

4. Select a peak detect algorithm in the Peak Detect list to specify how the data system finds and processes chromatogram peaks.

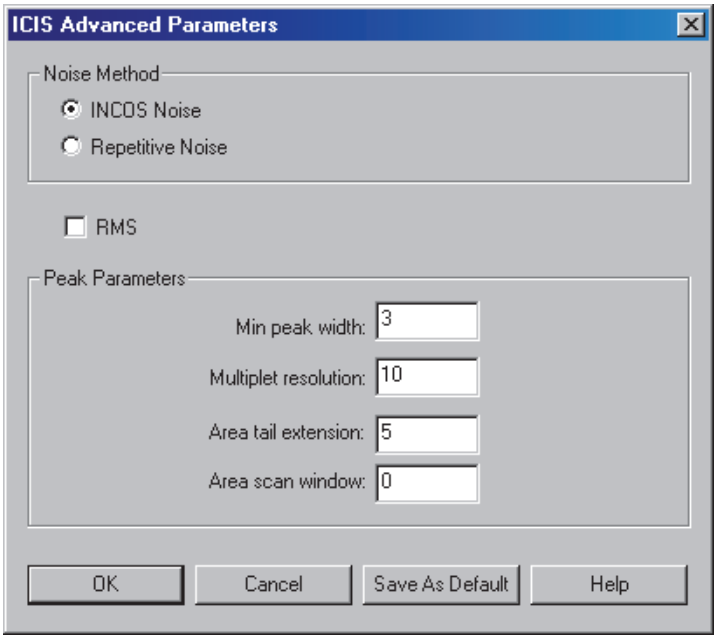
ICIS	This algorithm has been designed for MS data and has superior peak detection efficiency at low MS signal levels. This is the Xcalibur default peak detection algorithm.
Genesis	This algorithm is the original Xcalibur peak detection algorithm and has been provided for backward compatibility with Xcalibur 1.0 data system studies.
Avalon	This algorithm supports detectors other than MS and detects negative chromatographic peaks and shoulders more accurately than Genesis or ICIS.

5. In the Filter list, select a scan filter.
6. To accept current changes to the Identification page, click **OK**.
7. To set advanced parameters, click the **Advanced** button (see Figure 49).

Note For the following procedure, the ICIS Advanced Parameters dialog box opens. If you choose another peak detect method, a different Advanced Parameters dialog box opens. Fill in the values that are appropriate for the method.

a. Confirm that the **INCOS Noise** option is selected in the Noise Method area.

Figure 49. ICIS Advanced Parameters dialog box



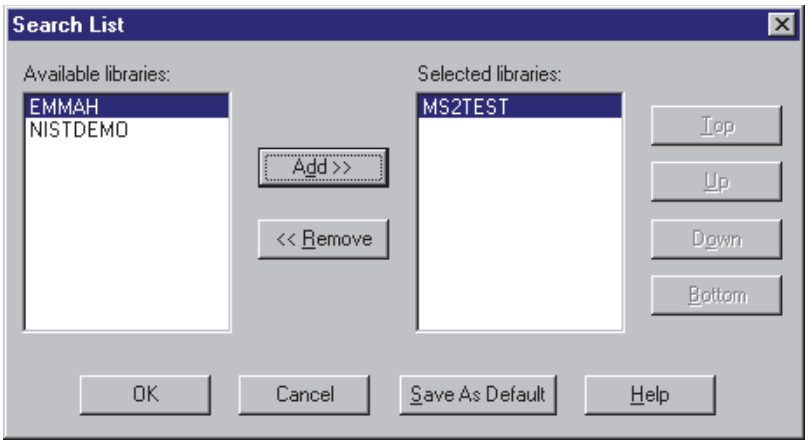
Note The Xcalibur data system generates the Available Libraries list dynamically. Each time you open the Search List dialog box, The application lists the libraries available on the system at that time.

Libraries listed in the Selected Libraries list, on the other hand, might not exist on the system. They might have been selected on another system or deleted or renamed since the processing method was created.

b. To close the dialog box and return to the Processing Setup window, click **OK**.

8. To apply changes to the Identification page, click **OK**.
9. Specify the name of the library to search:
   a. To display search type options, click the **Library Search Options** tab.
   b. To display the list of available libraries, click **Search List** (see Figure 50).

Figure 50. Search List dialog box



   c. To select a library to search, highlight the library name in the Available Libraries list and click **Add** to move the library name to the Selected Libraries list.
   d. Click **OK** to select that library and return to the Qual view of the Processing Setup window.

Specifying Report Options for Library Searches

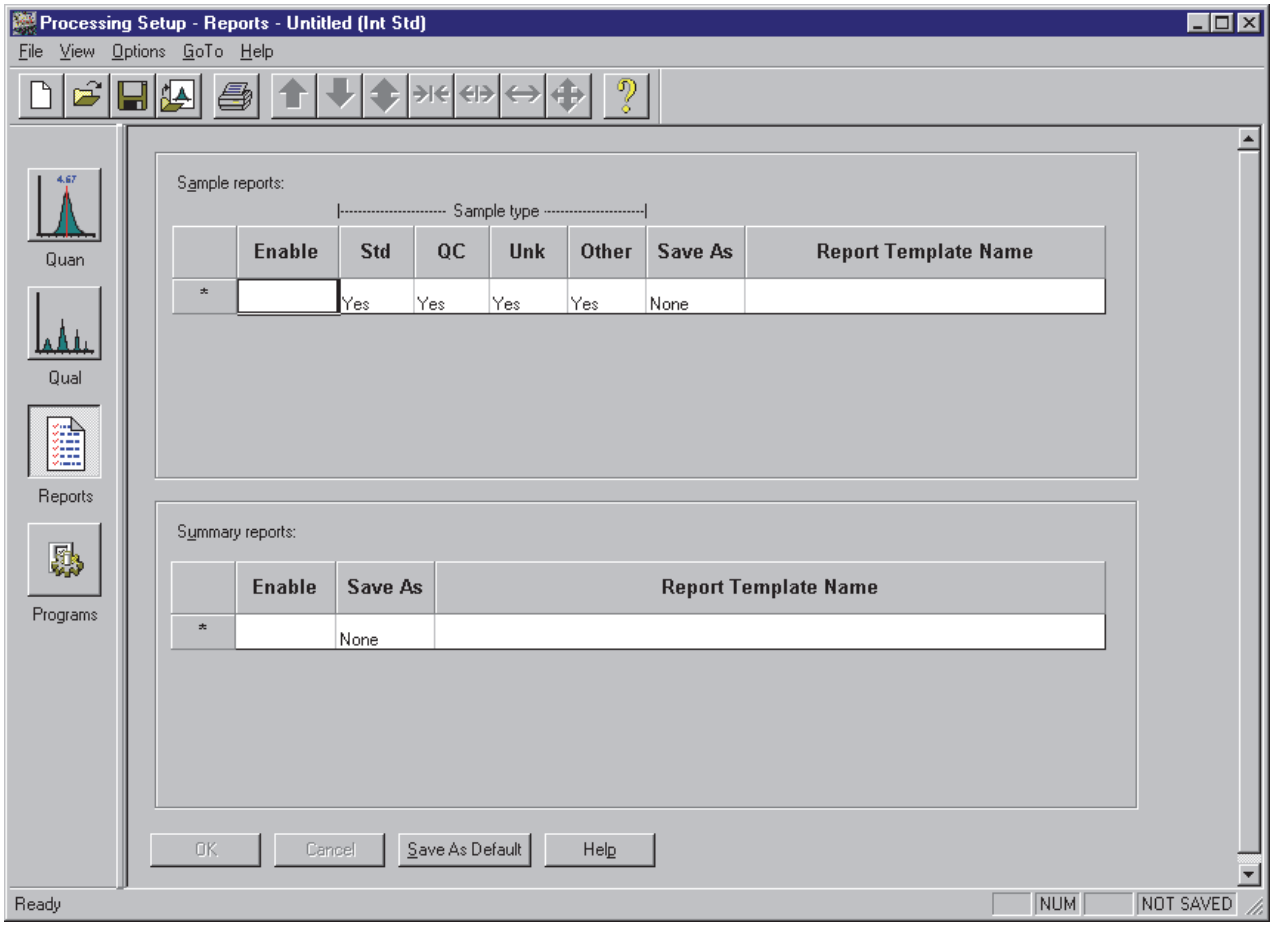
To produce and print reports automatically, specify report options from the Reports view of the Processing Setup window after specifying library search characteristics.

Note For more information about creating custom report templates using Microsoft™ Word, refer to the *XReport User Guide*.

❖ To display the raw file data in the format of a custom report template

1. Click on the View bar in the Processing Setup window or choose **View > Reports.** The Reports view appears (see Figure 51).

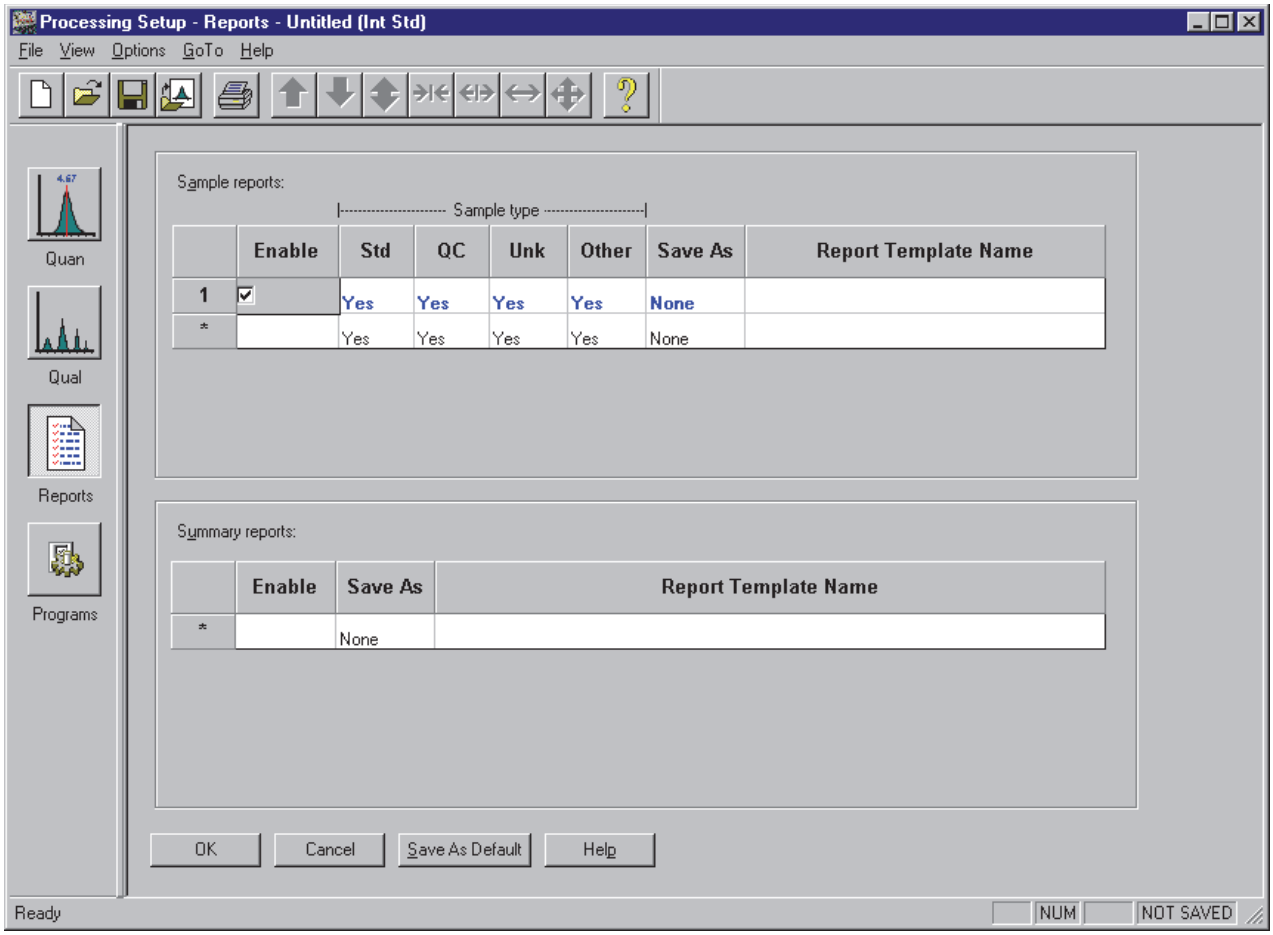
Figure 51. Reports view



2. If the Apply Changes? dialog box opens, read the ⚠ message and click **Yes**.

3. Click the **Enable** cell in the Sample Reports area. When a check box appears, select the check box to make Row 1 active (see Figure 52).

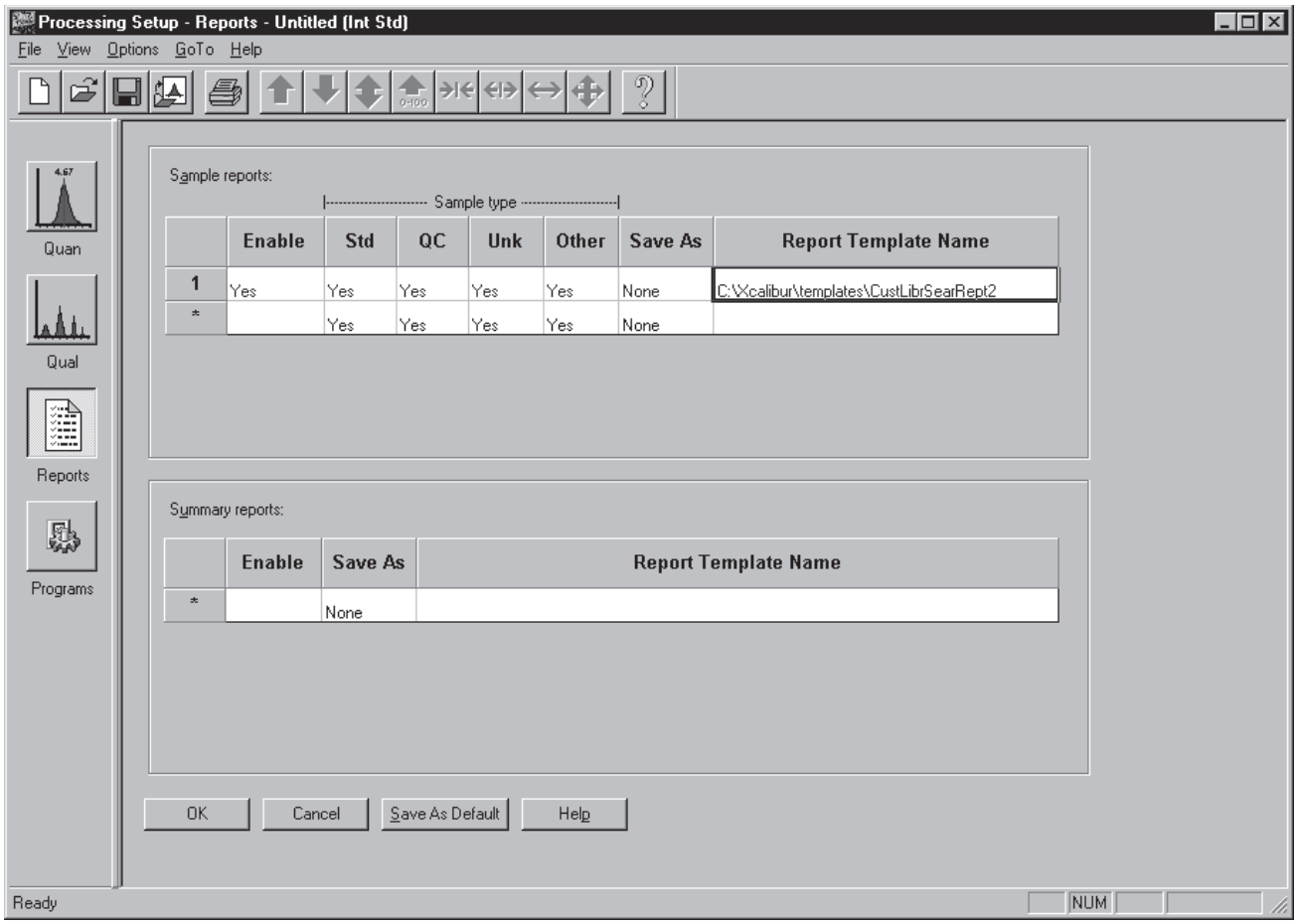
Figure 52. Reports view with Row 1 active



4. Specify the sample brackets in Row 1:
   a. To exclude the bracket for standards from the report, click **Yes** in the Std column and clear the check box.
   b. To exclude the bracket for quality control samples, click **Yes** in the QC column and clear the check box.
   c. Click **Yes** in the Other column and clear the check box.
5. Specify the name of a Report Template (.doc) in Row 1:
   a. To display the Browse for Sample Report Template dialog box, double-click the Report Template Name cell.
   b. Scroll to select a report template.
   c. To select the report template, and display the filename in the Report Template Name cell, click **Open**.

6. To apply changes to the Reports view, click **OK**. Figure 53 shows the Reports view and a specified Report Template Name.

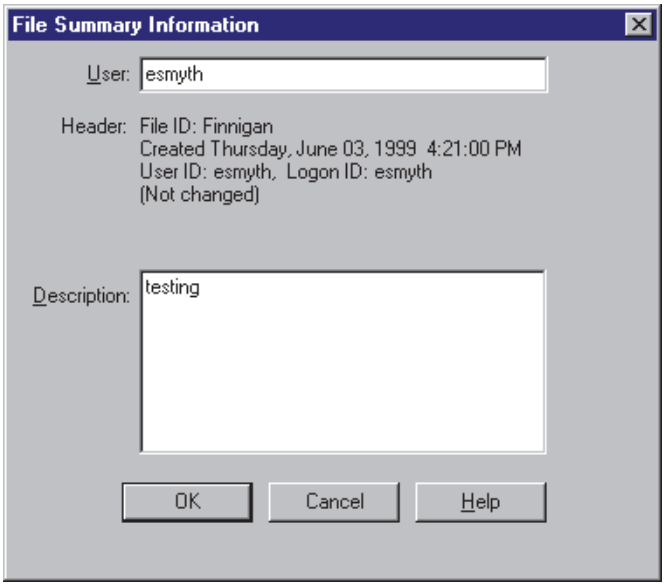
Figure 53. Processing Setup window



7. Save the processing method:

   a. Choose **File > Save As**. The File Summary Information dialog box opens (see Figure 54).

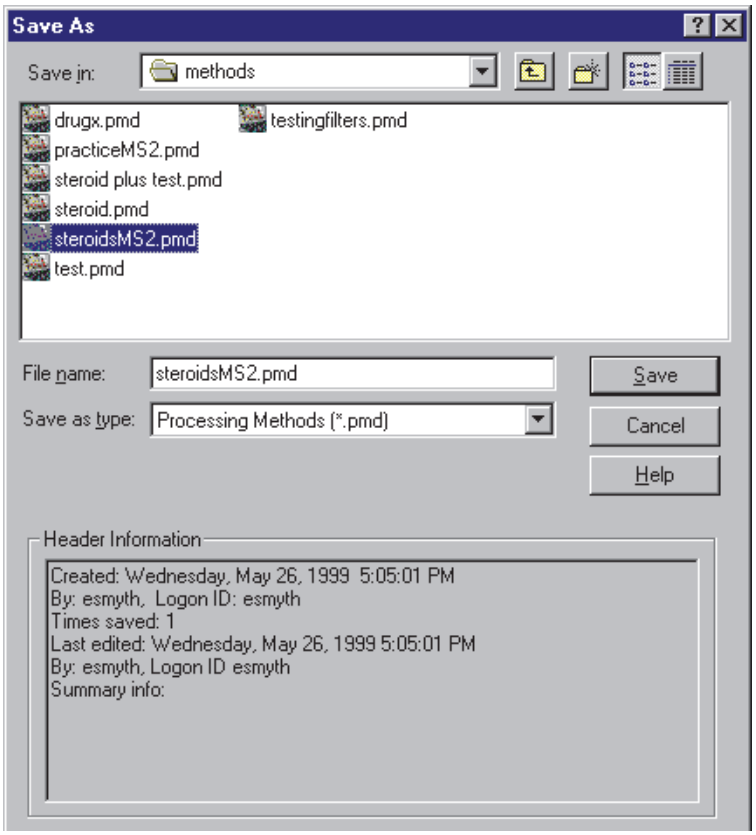
   Figure 54. File Summary Information dialog box



   b. Type file summary information in the Description box and click **OK**. The Save As dialog box opens.

c. In the Save As dialog box, type a name the processing method (see Figure 55).

Figure 55. Save As dialog box



d. To save the method and return to the Reports view, click **Save**.

8. To close the Processing Setup window and return to the Xcalibur Home Page, choose **File > Exit**.

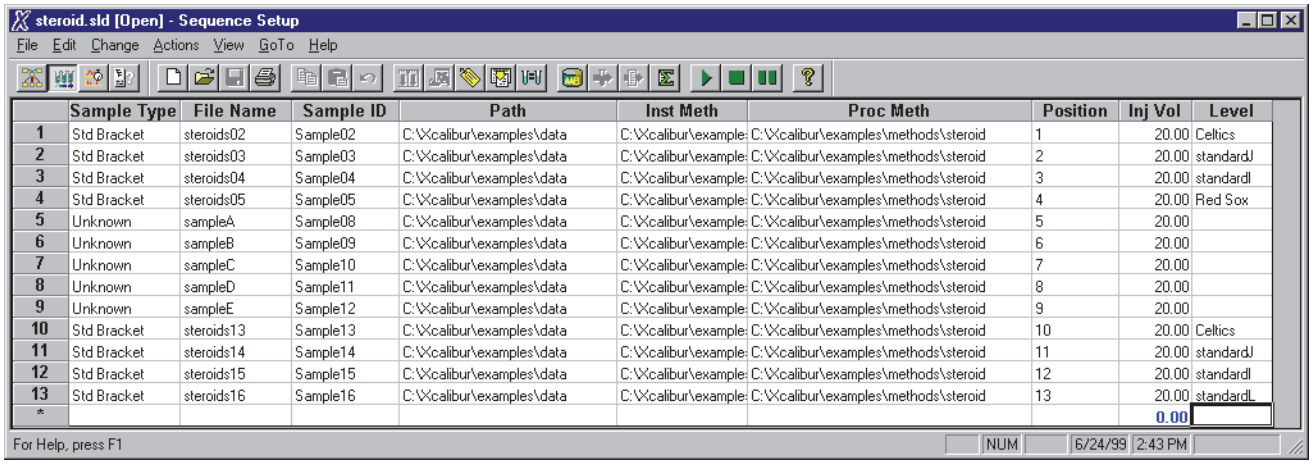
Specifying Raw Data Files in Sequence Setup

To search libraries and print reports automatically, specify the raw files containing the data to process.

❖ To display the Sequence Setup window and open a sequence list (.sld)

1. To display the Sequence Setup window, click on the Xcalibur Home Page.
2. To display the Open dialog box, choose **File > Open**.
3. Scroll to select a sequence file and double-click to display the list of samples (see Figure 56).

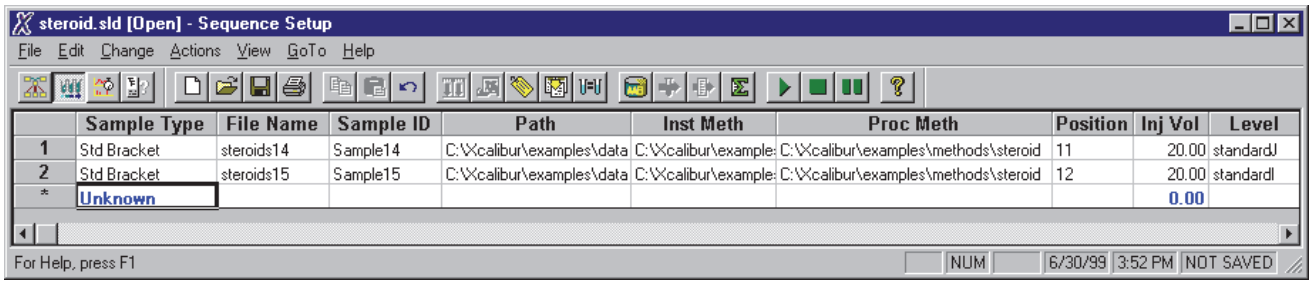
Figure 56. Sequence Setup window



	Sample Type	File Name	Sample ID	Path	Inst Meth	Proc Meth	Position	Inj Vol	Level
1	Std Bracket	steroids02	Sample02	C:\Xcalibur\examples\data	C:\Xcalibur\example	C:\Xcalibur\examples\methods\steroid	1	20.00	Celtics
2	Std Bracket	steroids03	Sample03	C:\Xcalibur\examples\data	C:\Xcalibur\example	C:\Xcalibur\examples\methods\steroid	2	20.00	standardJ
3	Std Bracket	steroids04	Sample04	C:\Xcalibur\examples\data	C:\Xcalibur\example	C:\Xcalibur\examples\methods\steroid	3	20.00	standardl
4	Std Bracket	steroids05	Sample05	C:\Xcalibur\examples\data	C:\Xcalibur\example	C:\Xcalibur\examples\methods\steroid	4	20.00	Red Sox
5	Unknown	sampleA	Sample08	C:\Xcalibur\examples\data	C:\Xcalibur\example	C:\Xcalibur\examples\methods\steroid	5	20.00	
6	Unknown	sampleB	Sample09	C:\Xcalibur\examples\data	C:\Xcalibur\example	C:\Xcalibur\examples\methods\steroid	6	20.00	
7	Unknown	sampleC	Sample10	C:\Xcalibur\examples\data	C:\Xcalibur\example	C:\Xcalibur\examples\methods\steroid	7	20.00	
8	Unknown	sampleD	Sample11	C:\Xcalibur\examples\data	C:\Xcalibur\example	C:\Xcalibur\examples\methods\steroid	8	20.00	
9	Unknown	sampleE	Sample12	C:\Xcalibur\examples\data	C:\Xcalibur\example	C:\Xcalibur\examples\methods\steroid	9	20.00	
10	Std Bracket	steroids13	Sample13	C:\Xcalibur\examples\data	C:\Xcalibur\example	C:\Xcalibur\examples\methods\steroid	10	20.00	Celtics
11	Std Bracket	steroids14	Sample14	C:\Xcalibur\examples\data	C:\Xcalibur\example	C:\Xcalibur\examples\methods\steroid	11	20.00	standardJ
12	Std Bracket	steroids15	Sample15	C:\Xcalibur\examples\data	C:\Xcalibur\example	C:\Xcalibur\examples\methods\steroid	12	20.00	standardl
13	Std Bracket	steroids16	Sample16	C:\Xcalibur\examples\data	C:\Xcalibur\example	C:\Xcalibur\examples\methods\steroid	13	20.00	standardL
*								0.00	

4. To exclude samples from the list, highlight rows to exclude and choose **Edit > Delete Row**. The data system displays a message box to confirm the Delete Row command. Click **Yes** (see Figure 57).

Figure 57. Sequence Setup window after excluding rows

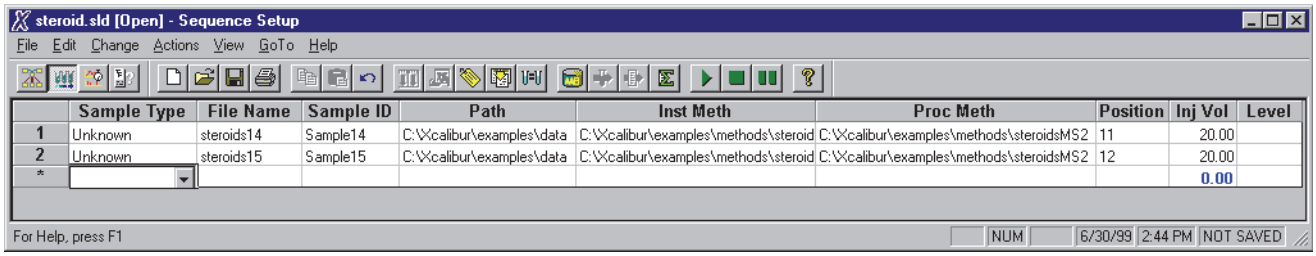


	Sample Type	File Name	Sample ID	Path	Inst Meth	Proc Meth	Position	Inj Vol	Level
1	Std Bracket	steroids14	Sample14	C:\Xcalibur\examples\data	C:\Xcalibur\example	C:\Xcalibur\examples\methods\steroid	11	20.00	standardJ
2	Std Bracket	steroids15	Sample15	C:\Xcalibur\examples\data	C:\Xcalibur\example	C:\Xcalibur\examples\methods\steroid	12	20.00	standardl
*	Unknown							0.00	

Note Use Sequence Setup to create a sequential list containing a variety of sample types or brackets. However, when performing qualitative analysis, the type is usually unknown.

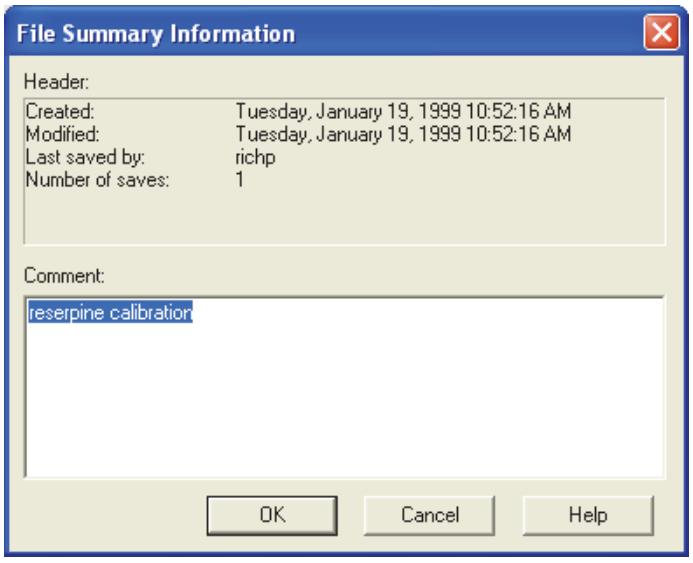
5. To view the Sample Type column, click the left side of the horizontal scroll bar at the bottom of the workspace. Double-click the Row 1 cell in the Sample Type column to display a drop-down list. Then, scroll up to select **Unknown**.
6. Expand the width of the Path column to confirm that the directory is the one storing the raw files. For example, raw files containing steroids data are found in C:\Xcalibur\examples\data.
7. To select the processing method, double-click the Row 1 cell in the Processing Method column. Browse to select the processing method. Figure 58 shows the edited list of two files contained in steroid.sld.

Figure 58. Sequence Setup window


steroid.sld [Open] - Sequence Setup
File Edit Change Actions View GoTo Help
Sample Type File Name Sample ID Path Inst Meth Proc Meth Position Inj Vol Level
1 Unknown steroids14 Sample14 C:\Xcalibur\examples\data C:\Xcalibur\examples\methods\steroid C:\Xcalibur\examples\methods\steroidsMS2 11 20.00
2 Unknown steroids15 Sample15 C:\Xcalibur\examples\data C:\Xcalibur\examples\methods\steroid C:\Xcalibur\examples\methods\steroidsMS2 12 20.00
* 0.00
For Help, press F1
NUM
6/30/99 2:44 PM NOT SAVED

8. Repeat Steps 4 and 5 for all other rows of the sequence. Step 6 is repeated automatically for subsequent rows.
9. To save the sequence list file, choose **File > Save As**. The File Summary Information dialog box opens. Type a description in the Comment box and click **OK**.

Figure 59. File Summary Information dialog box



The Save As dialog box opens.

10. Type a name in the File Name box to name the sequence.
11. Click **Save** to save the sequence list and return to the Sequence Setup window.

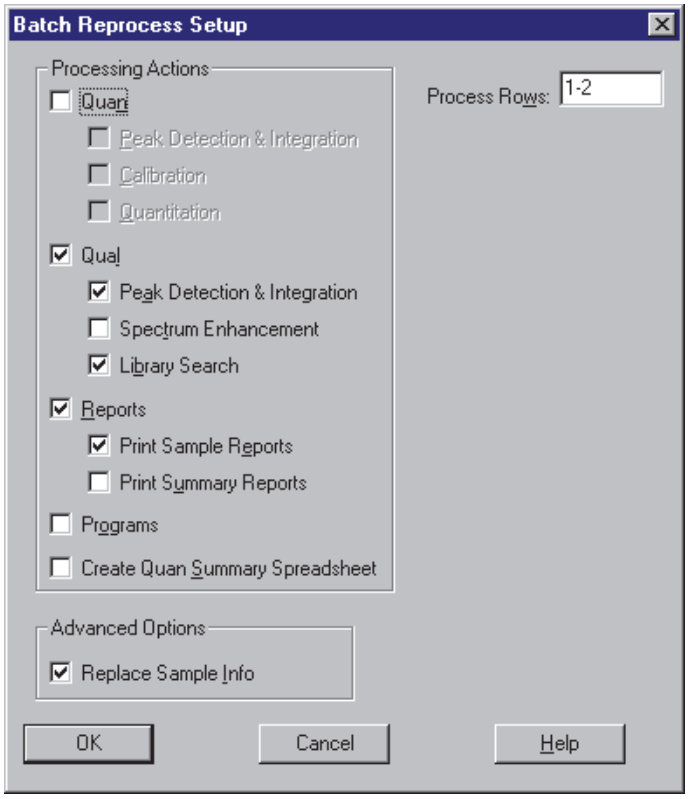
Processing Raw Files and Printing Reports

To batch process raw data and print reports automatically, use Sequence Setup. Whether you are processing or reprocessing the data, the results are the same. This guide refers to processed data whether the action is processing or reprocessing.

❖ To process a list of raw files and print library search reports

1. To display the Sequence Setup window, click on the Xcalibur Home Page.
2. To select the rows in the current sequence to process, in Sequence Setup, click and hold on the row number in the first row to process and drag the cursor to the bottom row. The data system highlights the selected rows.
3. Click on the tool bar or choose **Actions > Batch Reprocess**. The Batch Reprocess Setup dialog box opens (Figure 60).

Figure 60. Batch Reprocess Setup dialog box



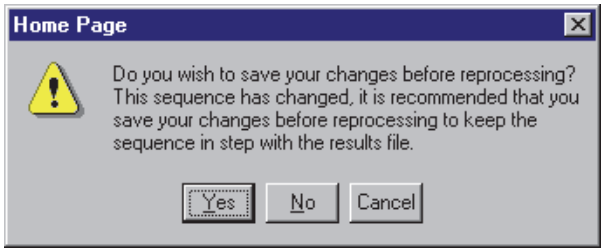
4. Confirm that the Process Rows box lists all row numbers (for example *1-2)*. If the numbers are missing, double-click the box and type the row numbers.

5. Select ☑ any of the following check boxes.

   - Quan
     - Peak Detection & Integration
     - Calibration
     - Quantitation
   - Qual
     - Peak Detection & Integration
     - Spectrum Enhancement
     - Library Search
   - Reports
     - Print Sample Reports
     - Print Summary Reports
   - Programs
   - Create Quan Summary Spreadsheet
   - Advanced Options
   - Replace Sample Info

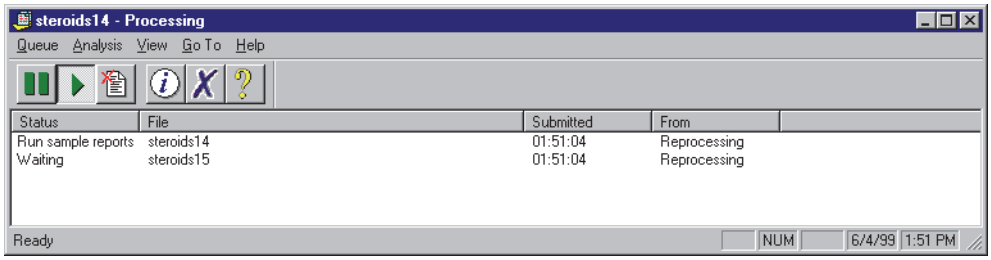
6. To initiate batch processing of the selected samples, click **OK**. If the data system displays a Save your changes box, as shown in Figure 61, click **Yes**.

Figure 61. Message box


Home Page
Do you wish to save your changes before reprocessing? This sequence has changed, it is recommended that you save your changes before reprocessing to keep the sequence in step with the results file.
Yes
No
Cancel

7. To display the Processing Status window (see Figure 62), click the **Queue Manager** task in your computer task bar.

Figure 62. Processing Status window



Two beeps signal the end of the batch processing.

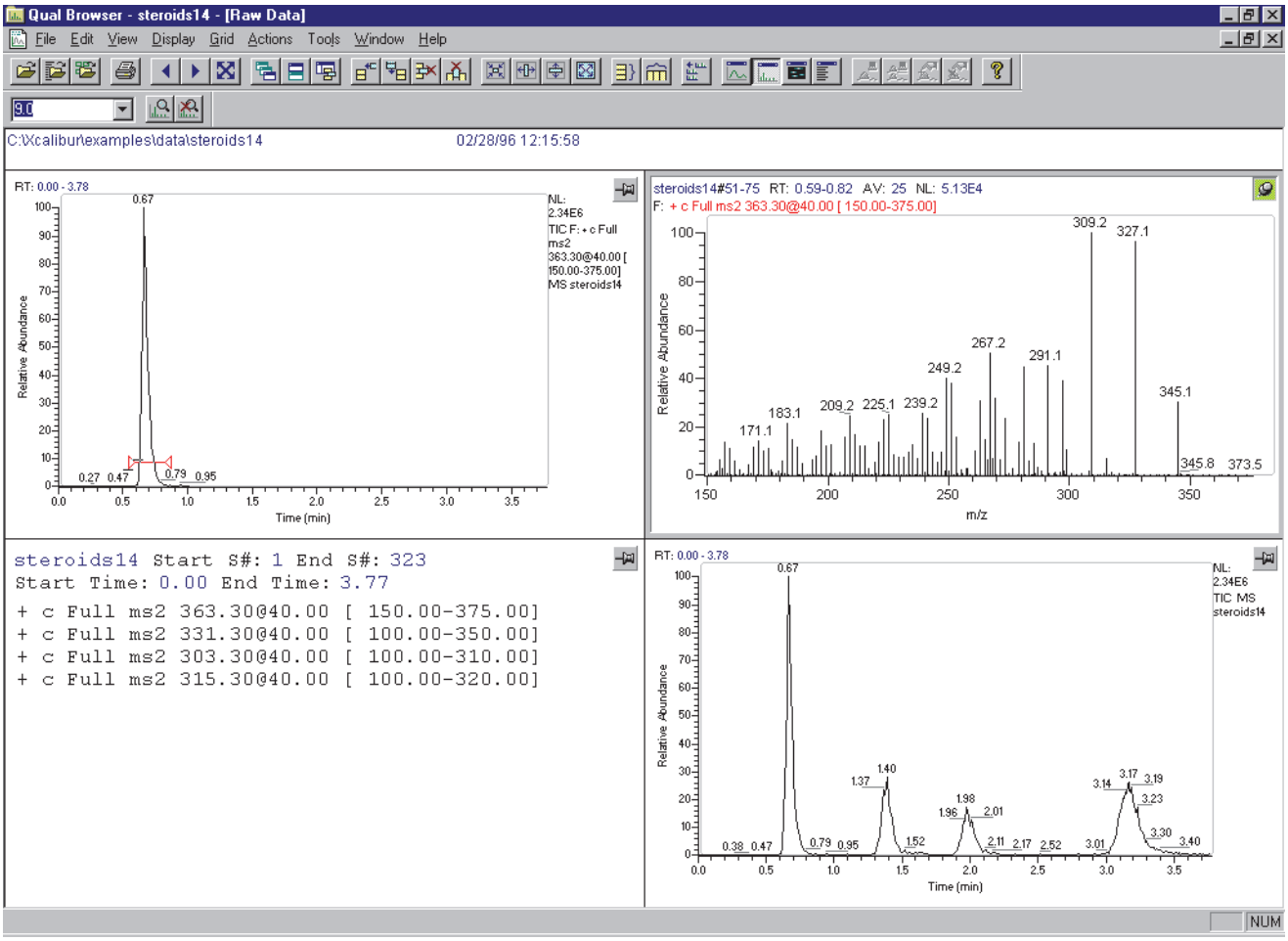
8. Check your printed reports to see that they provide the information you wanted.

Initiating a Library Search from Qual Browser

❖ **To perform a library search from the Qual Browser window**

1. Click on the Xcalibur Home Page to display the Qual Browser window.
2. To open a raw file that contains steroids data, choose **File > Open** or click in the toolbar. The Open Raw File dialog box opens.
3. Browse to a raw file and click **Open**.
4. View a spectrum. For procedure details, see "Viewing a Spectrum in Qual Browser" on page 16. Figure 63 shows four views (clockwise from lower left): Scan Filter view, (filtered) Chromatogram view, (averaged) Spectrum view, and (unfiltered) Chromatogram view.

Figure 63. Qual Browser window

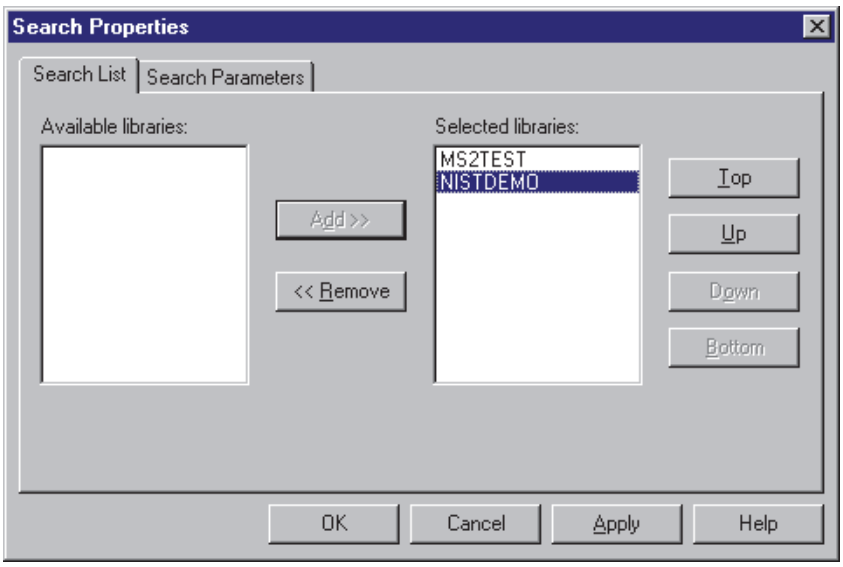

Qual Browser - steroids14 - [Raw Data]
File Edit View Display Grid Actions Tools Window Help
C:\Xcalibur\examples\data\steroids14
02/28/96 12:15:58
RT: 0.00 - 3.78
NL: 2.34E6 TIC F: + c Full ms2 363.30@40.00 [150.00-375.00] MS steroids14
Relative Abundance
Time (min)
steroids14#51-75 RT: 0.59-0.82 AV: 25 NL: 5.13E4
F: + c Full ms2 363.30@40.00 [150.00-375.00]
m/z
steroids14 Start S#: 1 End S#: 323
Start Time: 0.00 End Time: 3.77
+ c Full ms2 363.30@40.00 [150.00-375.00]
+ c Full ms2 331.30@40.00 [100.00-350.00]
+ c Full ms2 303.30@40.00 [100.00-310.00]
+ c Full ms2 315.30@40.00 [100.00-320.00]
RT: 0.00 - 3.78
NL: 2.34E6 TIC MS steroids14
NUM

5. Select one or more libraries to search:

   a. Right-click the Spectrum view (upper right). A shortcut menu appears.

   b. To display the Search Properties dialog box (see Figure 64), choose **Library > Options** from the shortcut menu.

   Figure 64. Search Properties dialog box with selected library



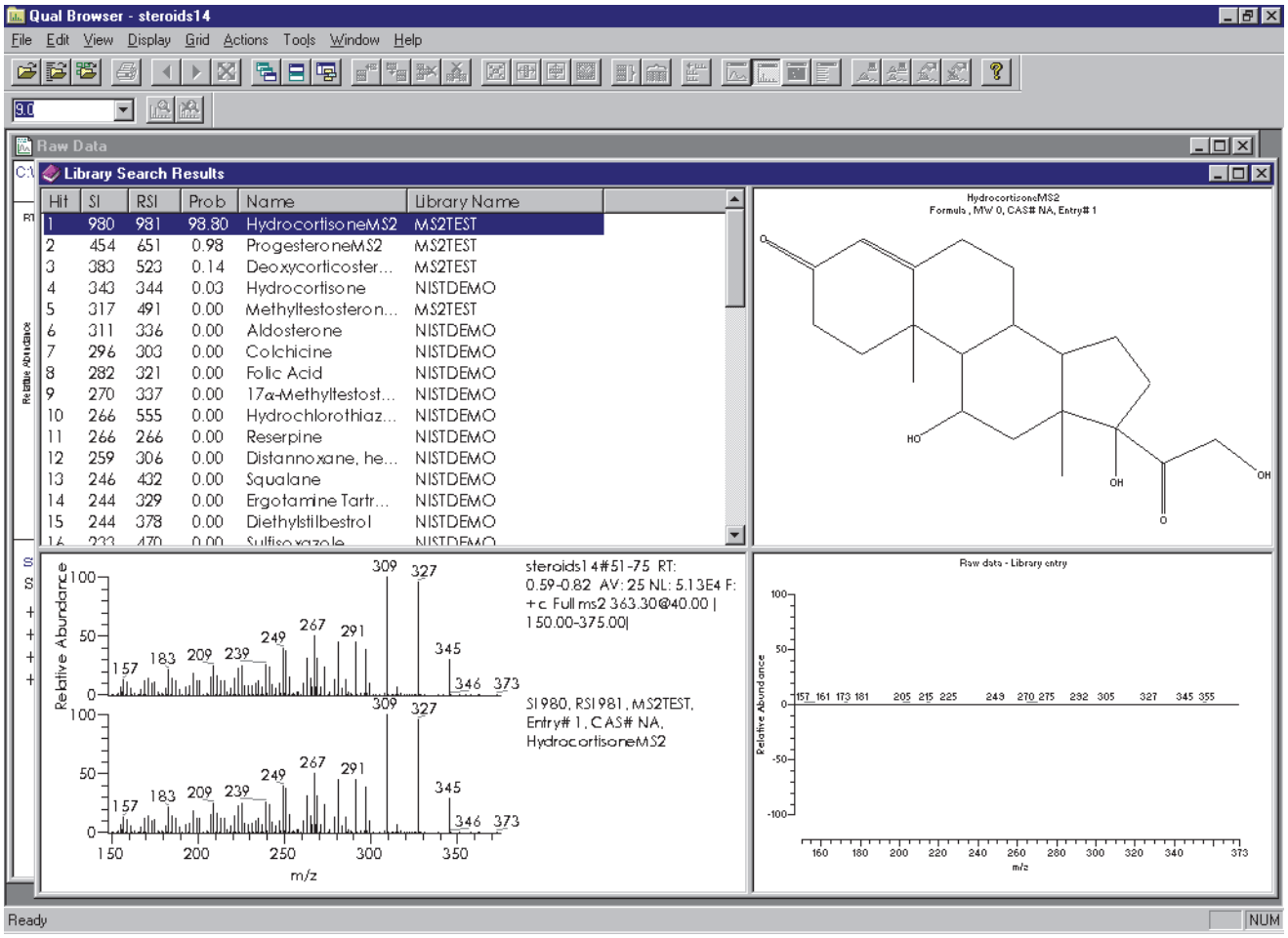
   c. Confirm that any libraries you want to search are listed in the Selected Libraries list.

   d. Click **OK** to save the settings, close the dialog box, and return to the Qual Browser window.

6. To start the library search, right-click the Spectrum view (upper right). From the shortcut menu, choose **Library > Search** to submit the spectrum to a library search.

   The data system displays library spectra (search results) that match the spectrum in a four-pane Library Search Results view (see Figure 65).

Figure 65. Library Search Results view cascaded with the Raw Data view


Qual Browser - steroids14
File Edit View Display Grid Actions Tools Window Help
Raw Data
Library Search Results
Hit SI RSI Prob Name Library Name
1 980 981 98.80 HydrocortisoneMS2 MS2TEST
2 454 651 0.98 ProgesteroneMS2 MS2TEST
3 383 523 0.14 Deoxycorticoster... MS2TEST
4 343 344 0.03 Hydrocortisone NISTDEMO
5 317 491 0.00 Methyltestosteron... MS2TEST
6 311 336 0.00 Aldosterone NISTDEMO
7 296 303 0.00 Colchicine NISTDEMO
8 282 321 0.00 Folic Acid NISTDEMO
9 270 337 0.00 17α-Methyltestost... NISTDEMO
10 266 555 0.00 Hydrochlorothiaz... NISTDEMO
11 266 266 0.00 Reserpine NISTDEMO
12 259 306 0.00 Distannoxane, he... NISTDEMO
13 246 432 0.00 Squalane NISTDEMO
14 244 329 0.00 Ergotamine Tartr... NISTDEMO
15 244 378 0.00 Diethylstilbestrol NISTDEMO
HydrocortisoneMS2
Formula , MW 0, CAS# NA, Entry# 1
steroids14#51-75 RT: 0.59-0.82 AV: 25 NL: 5.13E4 F: + c Full ms2 363.30@40.00 [150.00-375.00]
SI 980, RSI 981, MS2TEST, Entry# 1, CAS# NA, HydrocortisoneMS2
Raw data - Library entry
Relative Abundance
m/z
Ready
NUM

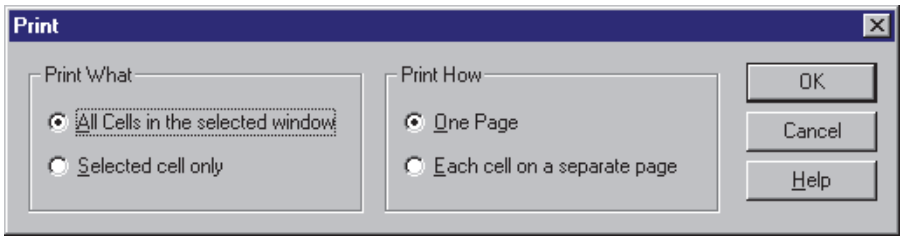
The interactive cells of the Library Search Results view show the following library search results, displayed clockwise from the upper left quadrant:

- Hits list (search results)
- Molecular structure, including formula, molecular weight, name, and library index number
- Difference spectrum (*Raw Data minus Library Entry*)
  - Peaks above the X-axis are relatively more intense in the spectrum than in the library entry.
  - Peaks below the X-axis are relatively more intense in the library entry than in the sample spectrum.

- Comparison of the sample spectrum and the library entry

7. To print the library search report, choose **File > Print Preview**. The Print dialog box opens (see Figure 66).

Figure 66. Print dialog box



8. Select options for your print display.
9. To close the dialog box and preview the results, click **OK**.
10. To display the Print dialog box again, click **Print** and click **OK**.
11. Click **OK** in the second Print dialog box to print the results. See "Library Sample Reports" on page 87 for an example of library search results initiated from Qual Browser.
12. Click to close the Library Search Results view.

Searching a Library Using Library Browser

To search a library, use the Library Browser window.

❖ To perform a library search on a spectrum exported from Qual Browser

1. Click in the Spectrum view (upper right) in the Qual Browser window to activate the window.
2. Right-click the Spectrum view to display the shortcut menu.

> **Note** To display data files in Library Browser, export them from Qual Browser. You can export a spectrum into Library Browser from Qual Browser after opening a raw file (.raw) or a result file (.rst) in Qual Browser.

3. Choose **Library > Export to Library Browser** to open the Library Browser windows automatically.

   When you export a spectrum to Library Browser, the data system automatically does the following:

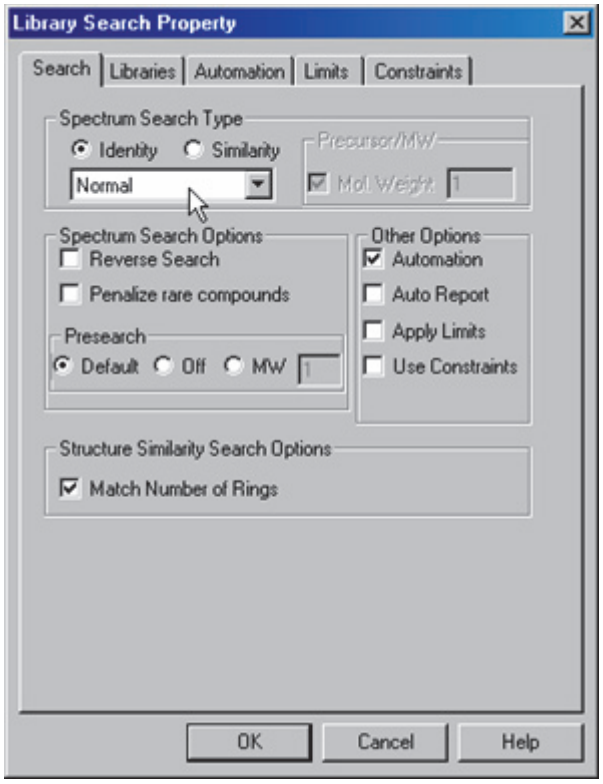
   - Copies information about the exported spectrum into the C:\Xcalibur\Libspecs directory. The data system gives the file an extension of .msd and truncates the filename to the first eight characters of the original filename.
   - Creates an index file containing details about the exported spectrum.

When Library Browser opens, the Xcalibur data system automatically does the following:

- Picks up the index file.
- Locates the exported .msd spectrum files and lists them in the Spec List pane.

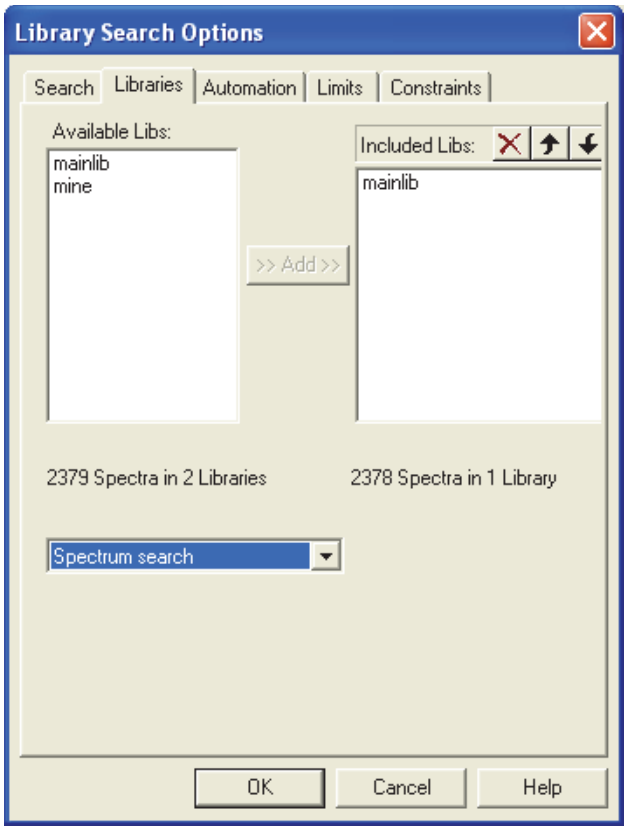
4. To define search parameters in Library Browser, choose **Tools > Library Search Options** to display the Library Search Property dialog box (see Figure 67).

Figure 67. Library Search Property dialog box



5. Click the **Libraries** tab to display the list of available and included libraries (see Figure 68). Use this dialog box to specify which libraries to search and the search order.

Figure 68. Libraries dialog box

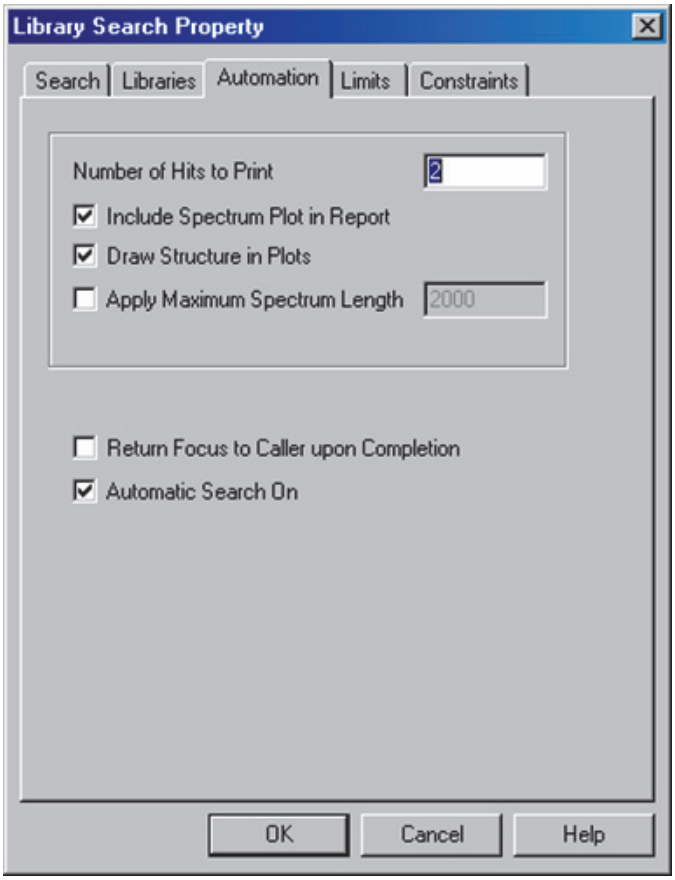


- To add a library to the search list, select its name in the Available Libs list and click **Add**.
- To exclude a library from the search list, select its name in the Included Libs list and click ✕.
- Click the **Search** tab and observe the *Automation* check box in the Other Options area (Figure 67).
- If the check box is checked for *Automation*, go to Step 5b save the parameters and close the Library Search Options dialog box.
- If the check box is not checked, go to Step 5a to set automation options.

a. To set automation options for searches, click the **Automation** tab and select the Automatic Search On check box.

The following figure shows possible settings for the option to automatically search libraries when exporting spectra to Library Browser.

Figure 69. Automation page



b. Click **OK** to save your options, close the dialog box, and return to the Library Browser windows. This action sets automatic searching as the default option the next time you open the Library Browser.

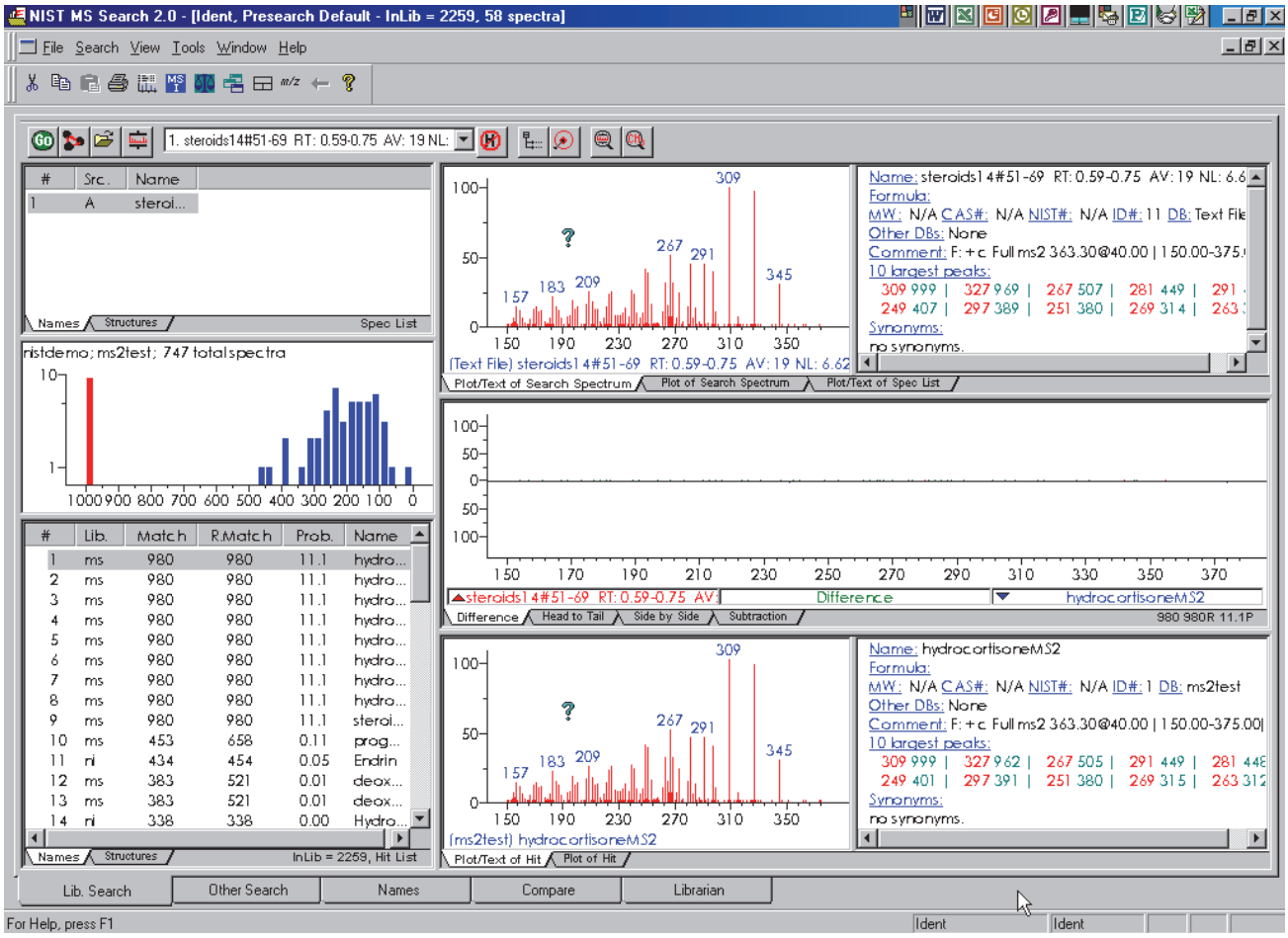
6. Double-click the entry in the Spec List pane to begin a library search. The interactive panes of Library Browser change to display the results of the search (see Figure 70).

- Hit List History drop-down list shows the results of the search.
- Hit List pane contains a list of spectral results.
- Structures panes (tab) display the chemical structure of the compound associated with the highlighted entry.
- Text panes display compound names, a mass/intensity list, and a scan filter of the highlighted entry.
- Plot panes display a single mass spectrum of a selected entry.

- Compare pane displays the difference between two spectra and presents them in various ways.

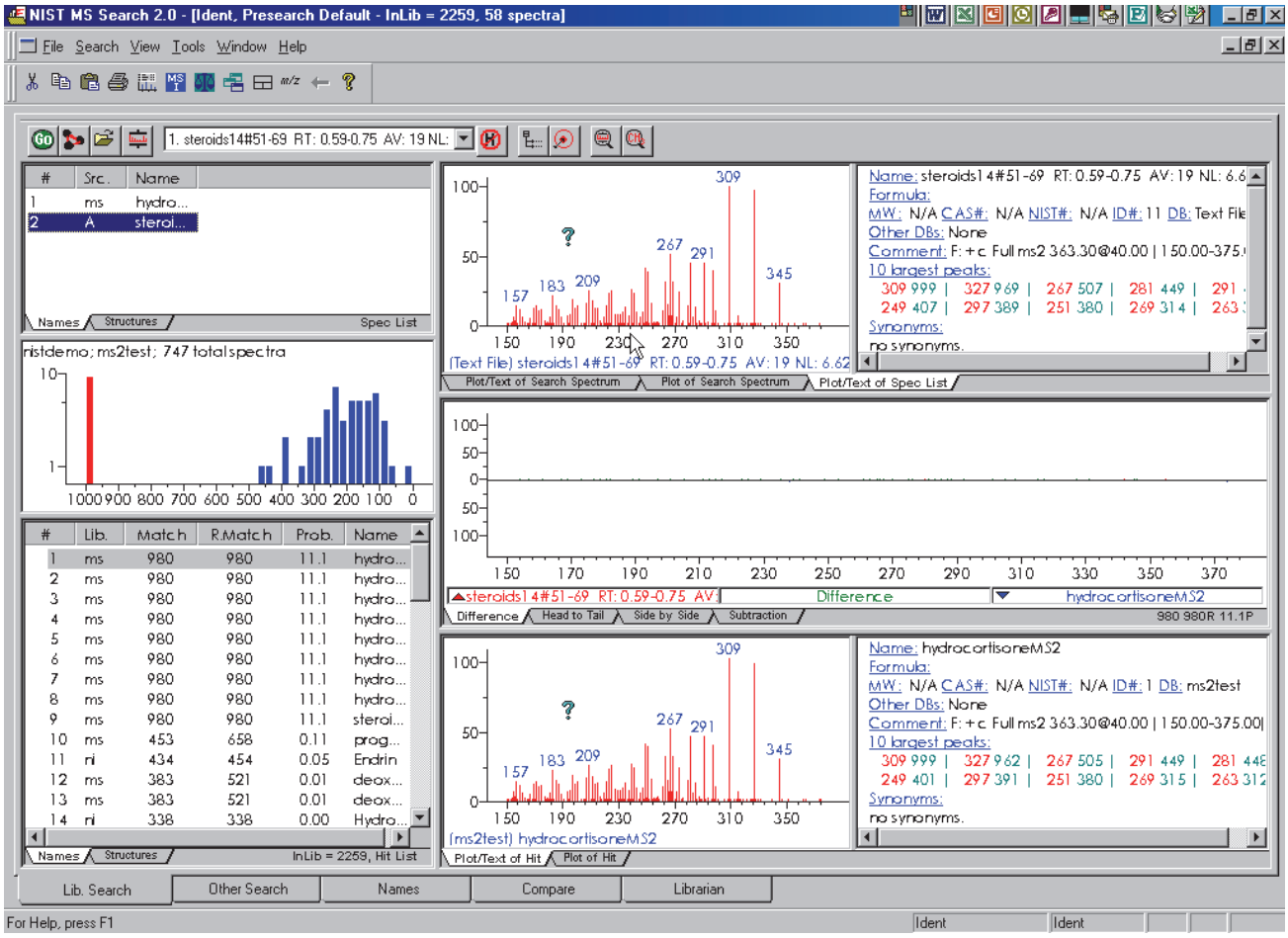
The following figure shows the library search results for a raw spectrum.

Figure 70. Library Browser default window


NIST MS Search 2.0 - [Ident, Presearch Default - InLib = 2259, 58 spectra]
File Search View Tools Window Help
1. steroids14#51-69 RT: 0.59-0.75 AV: 19 NL:
Src. Name
1 A steroi...
Names Structures Spec List
nistdemo; ms2test; 747 total spectra
Lib. Match R.Match Prob. Name
1 ms 980 980 11.1 hydro...
2 ms 980 980 11.1 hydro...
3 ms 980 980 11.1 hydro...
4 ms 980 980 11.1 hydro...
5 ms 980 980 11.1 hydro...
6 ms 980 980 11.1 hydro...
7 ms 980 980 11.1 hydro...
8 ms 980 980 11.1 hydro...
9 ms 980 980 11.1 steroi...
10 ms 453 658 0.11 prog...
11 ni 434 454 0.05 Endrin
12 ms 383 521 0.01 deox...
13 ms 383 521 0.01 deox...
14 ni 338 338 0.00 Hydro...
Names Structures InLib = 2259, Hit List
(Text File) steroids14#51-69 RT: 0.59-0.75 AV: 19 NL: 6.62
Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List
Name: steroids14#51-69 RT: 0.59-0.75 AV: 19 NL: 6.6
Formula:
MW: N/A CAS#: N/A NIST#: N/A ID#: 11 DB: Text File
Other DBs: None
Comment: F: + c Full ms2 363.30@40.00 [150.00-375.
10 largest peaks:
309 999 | 327 969 | 267 507 | 281 449 | 291
249 407 | 297 389 | 251 380 | 269 314 | 263
Synonyms:
no synonyms.
steroids14#51-69 RT: 0.59-0.75 AV:
Difference
hydrocortisoneMS2
Difference Head to Tail Side by Side Subtraction
980 980R 11.1P
(ms2test) hydrocortisoneMS2
Plot/Text of Hit Plot of Hit
Name: hydrocortisoneMS2
Formula:
MW: N/A CAS#: N/A NIST#: N/A ID#: 1 DB: ms2test
Other DBs: None
Comment: F: + c Full ms2 363.30@40.00 [150.00-375.00
10 largest peaks:
309 999 | 327 962 | 267 505 | 291 449 | 281 44
249 401 | 297 391 | 251 380 | 269 315 | 263 31
Synonyms:
no synonyms.
Lib. Search
Other Search
Names
Compare
Librarian
For Help, press F1
Ident
Ident

7. Right-click an entry in the Hit List pane to copy it to the first position in the Spec List pane (see Figure 71).

Figure 71. Library Browser default window, showing file copying from Hit List to Spec List panes


NIST MS Search 2.0 - [Ident, Presearch Default - InLib = 2259, 58 spectra]
File Search View Tools Window Help
1. steroids14#51-69 RT: 0.59-0.75 AV: 19 NL:
Lib. Search
Other Search
Names
Compare
Librarian
For Help, press F1

8. To print the search results, click **Print** in the tool bar. See "Library Sample Reports" on page 87 for an example of library search results initiated from Library Browser.

Library Sample Reports

This appendix contains samples of possible results using Xcalibur Library Browser.

Contents

- Reports from a Library Search Using Sequence Setup
- Report from a Library Search Using Qual Browser
- Report from a Library Search Using Library Browser

Reports from a Library Search Using Sequence Setup

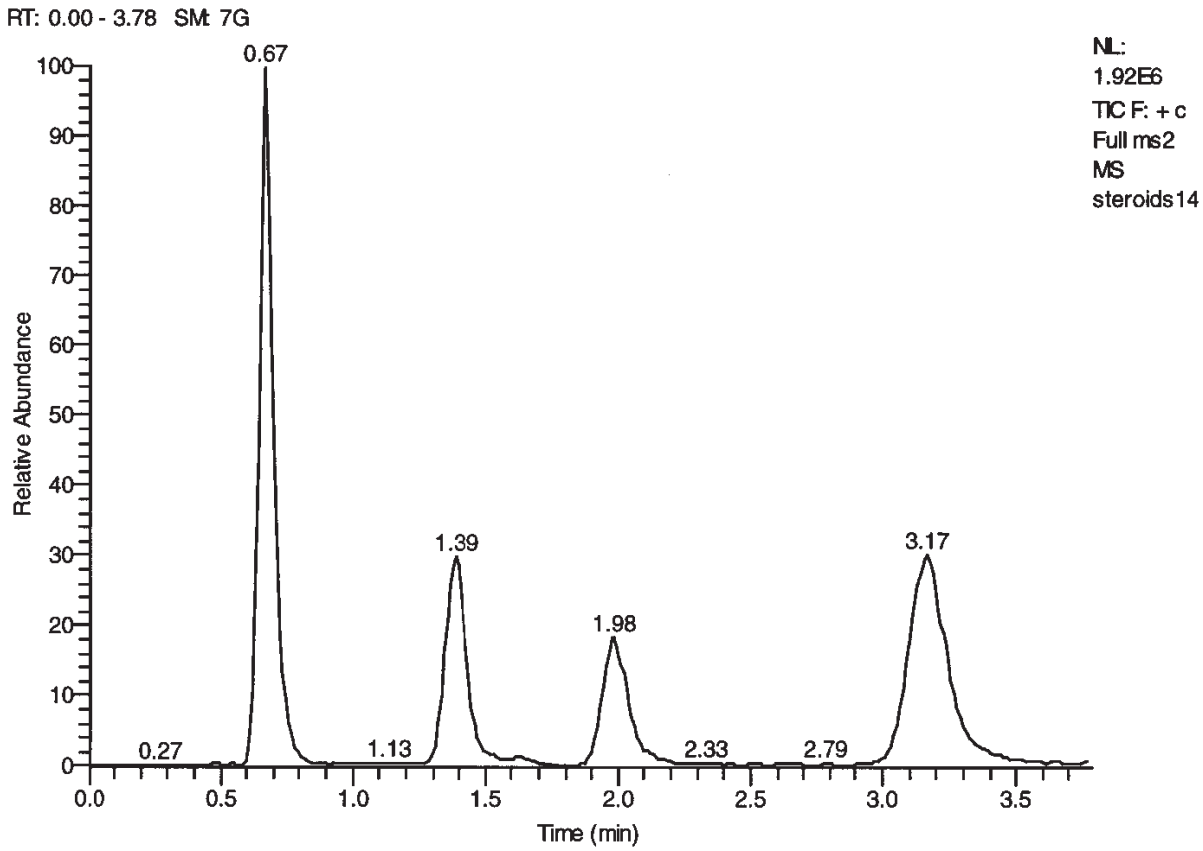
The Xcalibur data system prints reports library search reports automatically from Sequence Setup. Click the report name to view an example report:

- Library Search Report #1
  - Spectrum of Raw Data #1
  - Spectrum of Raw Data #2
  - Spectrum of Raw Data #3
  - Spectrum of Raw Data #4
- Library Search Report #2
  - Spectrum of Raw Data #1
  - Spectrum of Raw Data #2
  - Spectrum of Raw Data #3
  - Spectrum of Raw Data #4

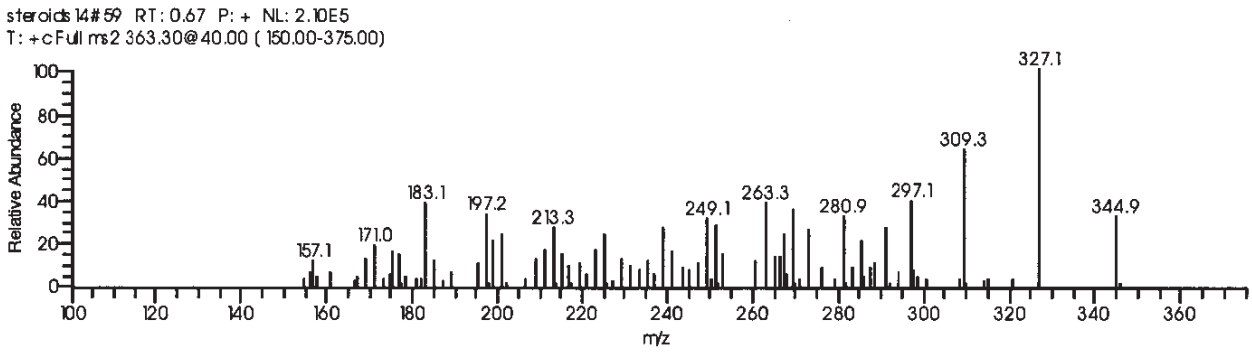
Library Search Report

Sample Name:	**Sample14**			Operator:	jackc
Acquisition Date:	02/28/96	Run Time (min):	3.78	Scans:	323
Acquisition Time:	12:15:58	Dil Factor:	1.00	Revision:	1.1 beta 1b
Low Mass (m/z):	100.00	High Mass (m/z):	375.00	Vial:	11
Samp Vol:	0.00	Samp Wt:	0.00	Inj Vol (uL):	20.00
Comments:					
Inst Method:	C:\pitcon\trial2\steroidMSMSis				
Proc Method:	C:\pitcon\trial2\				
Data Path:	C:\pitcon\trial2\steroidMSMSis				

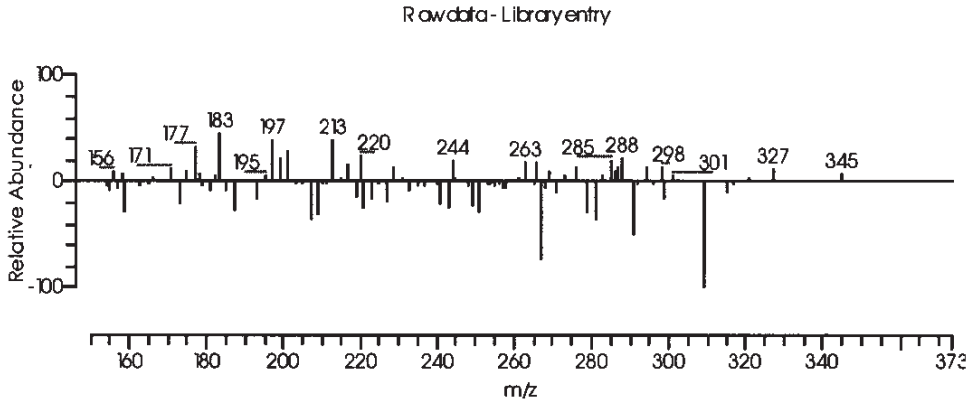
Qualitative Peaks



Spectrum of Raw Data



Difference Spectra



Library Spectrum of Most Probable Hit

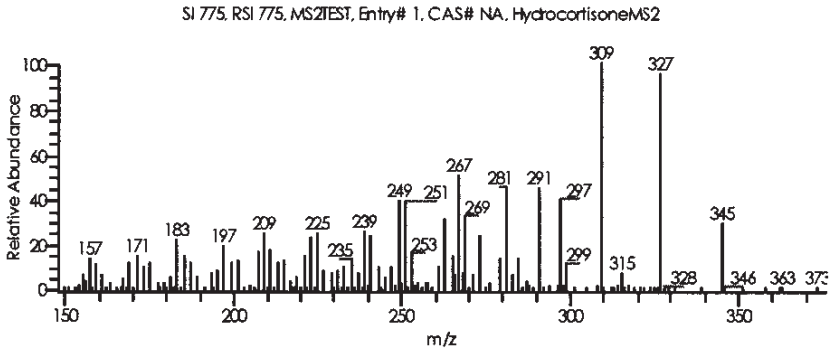
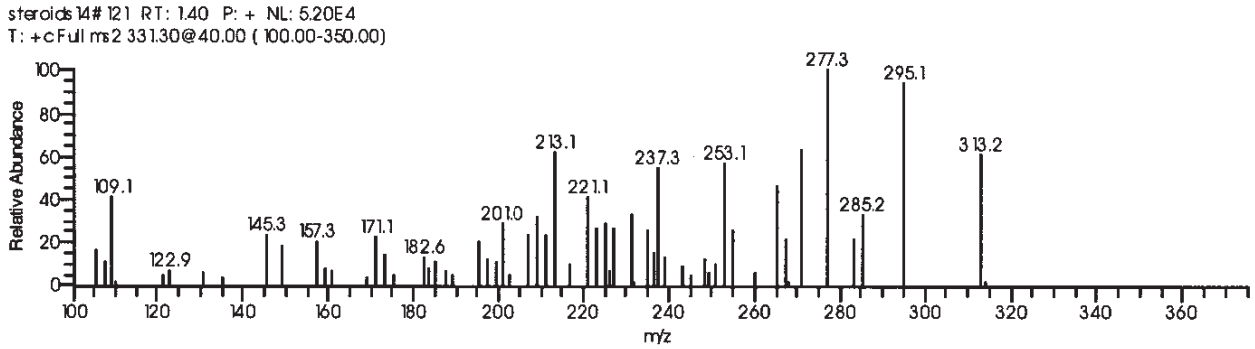


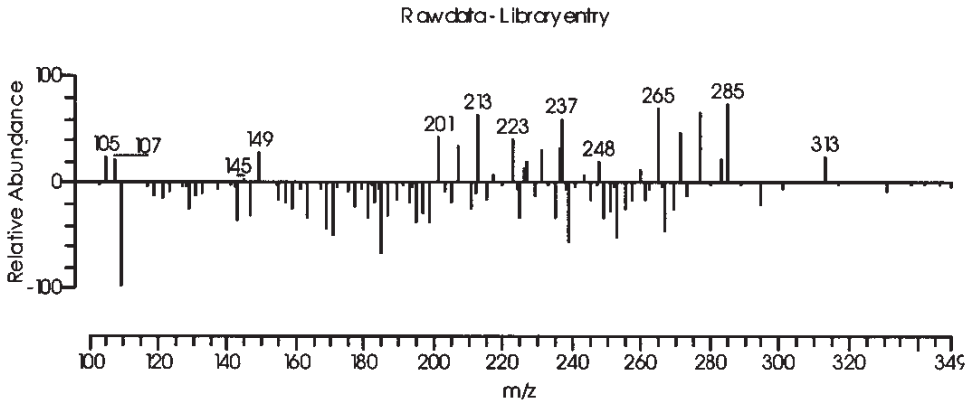
Table of Results

RT	Scan #	Probability, %	Name	SI	RSI	CAS #
0.67	59	98.76	HydrocortisoneMS2	775	775	NA
0.67	59	0.98	ProgesteroneMS2	374	551	NA
0.67	59	0.20	DeoxycorticosteroneMS2	325	461	NA
0.67	59	0.00	MethyltestosteroneMS2	275	424	NA

Spectrum of Raw Data



Difference Spectra



Library Spectrum of Most Probable Hit

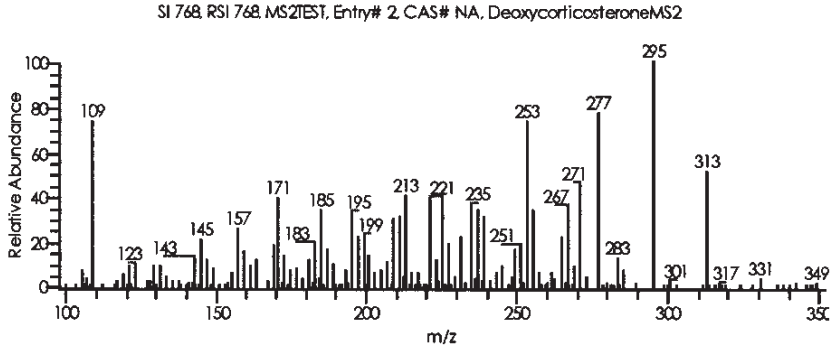
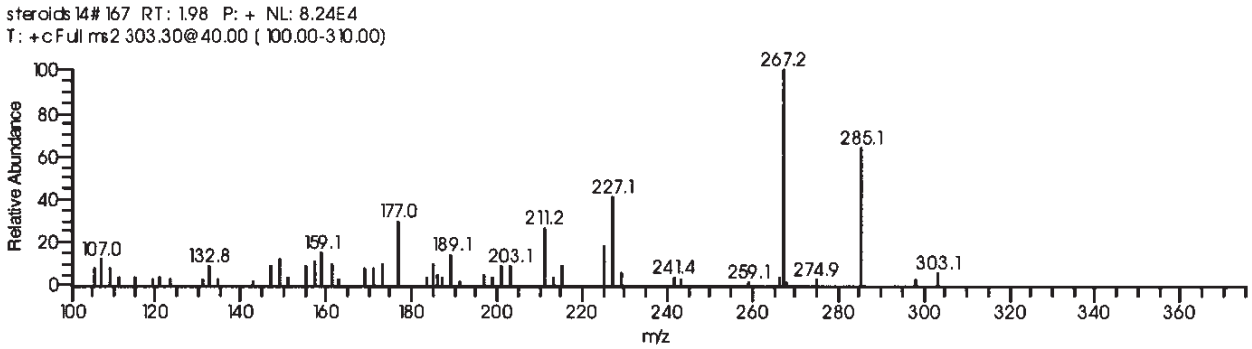


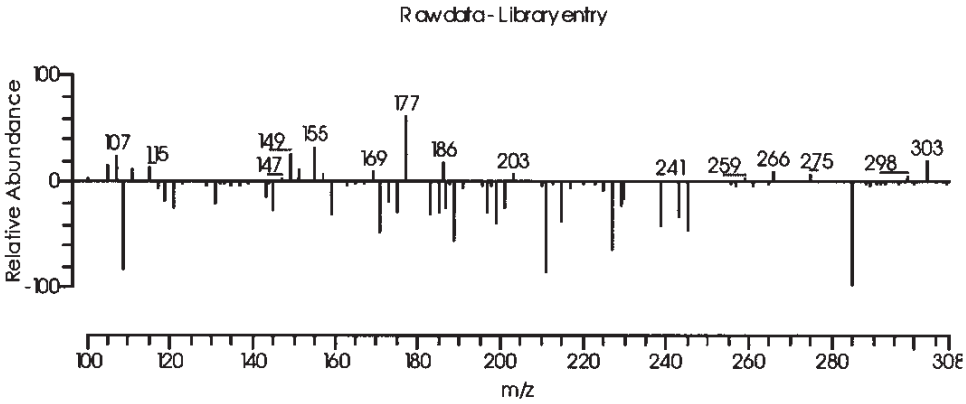
Table of Results

RT	Scan #	Probability, %	Name	SI	RSI	CAS #
1.40	121	97.83	DeoxycorticosteroneMS2	768	768	NA
1.40	121	0.97	HydrocortisoneMS2	331	375	NA
1.40	121	0.67	ProgesteroneMS2	320	367	NA
1.40	121	0.00	MethyltestosteroneMS2	313	434	NA

Spectrum of Raw Data



Difference Spectra



Library Spectrum of Most Probable Hit

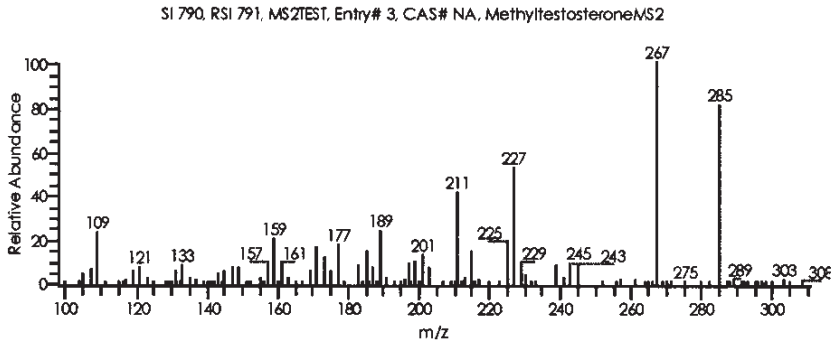
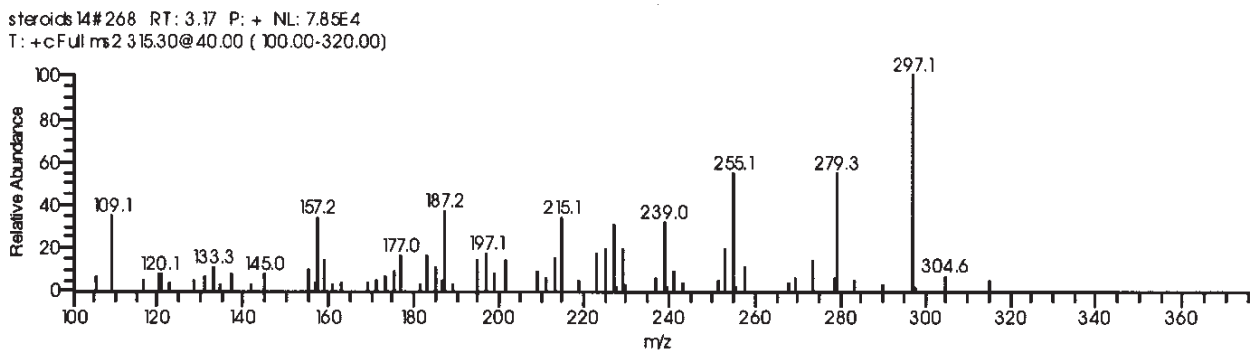


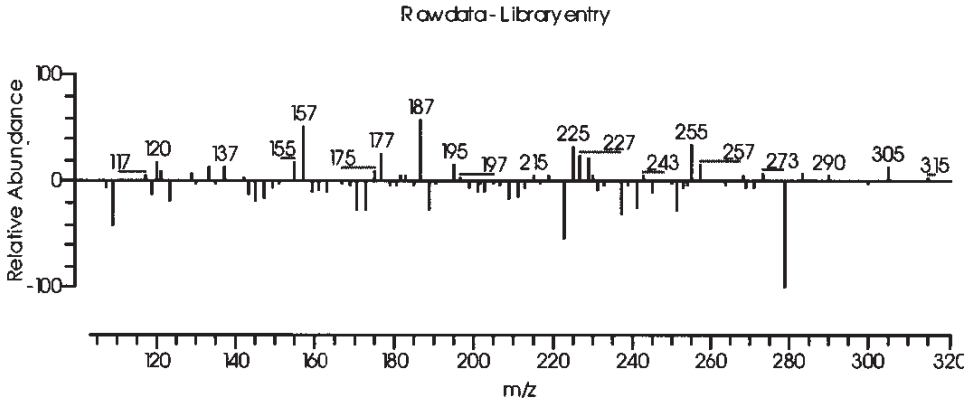
Table of Results

RT	Scan #	Probability, %	Name	SI	RSI	CAS #
1.98	167	98.58	MethyltestosteroneMS2	790	791	NA
1.98	167	0.98	DeoxycorticosteroneMS2	313	315	NA
1.98	167	0.33	HydrocortisoneMS2	289	292	NA
1.98	167	0.00	ProgesteroneMS2	264	347	NA

Spectrum of Raw Data



Difference Spectra



Library Spectrum of Most Probable Hit

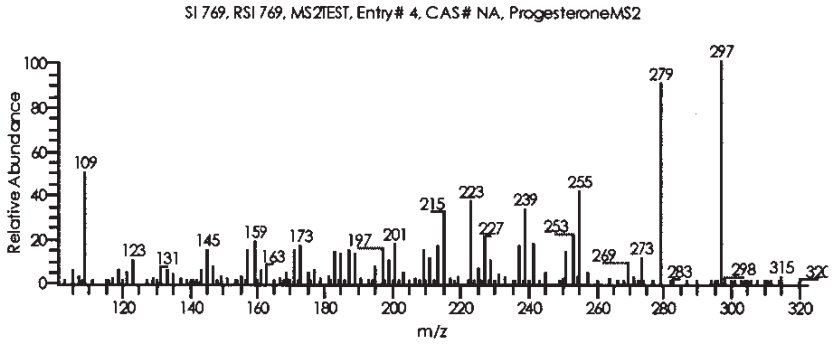


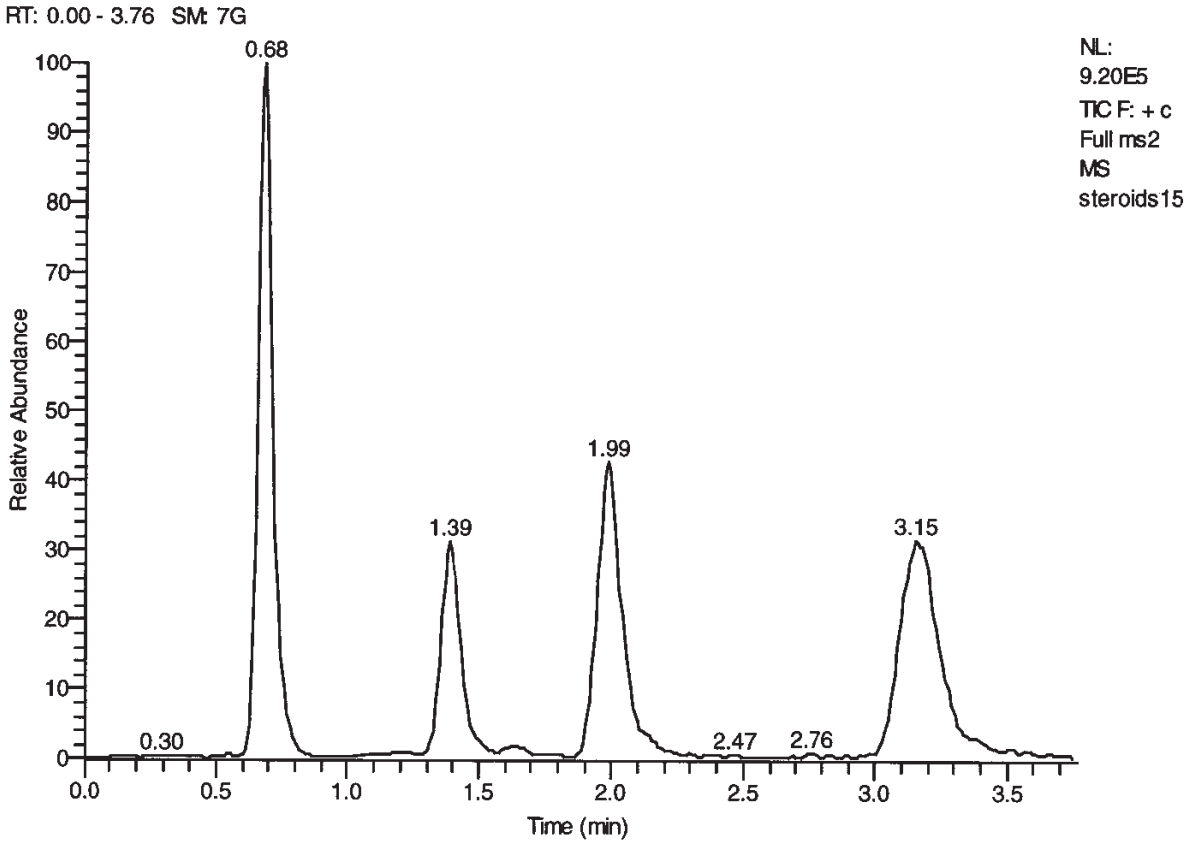
Table of Results

RT	Scan #	Probability, %	Name	SI	RSI	CAS #
3.17	268	98.61	ProgesteroneMS2	769	769	NA
3.17	268	0.98	HydrocortisoneMS2	403	404	NA
3.17	268	0.33	DeoxycorticosteroneMS2	379	463	NA
3.17	268	0.00	MethyltestosteroneMS2	329	386	NA

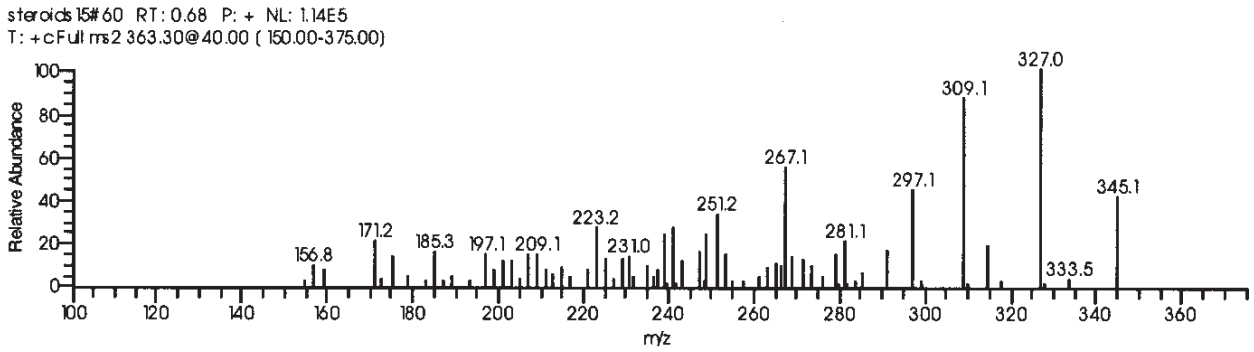
Library Search Report

Sample Name:	**Sample15**			Operator:	jackc
Acquisition Date:	02/28/96	Run Time (min):	3.75	Scans:	313
Acquisition Time:	12:21:31	Dil Factor:	1.00	Revision:	1.1 beta 1b
Low Mass (m/z):	100.00	High Mass (m/z):	375.00	Vial:	12
Samp Vol:	0.00	Samp Wt:	0.00	Inj Vol (uL):	20.00
Comments:					
Inst Method:	C:\pitcon\trial2\steroidMSMSis				
Proc Method:	C:\pitcon\trial2\				
Data Path:	C:\pitcon\trial2\steroidMSMSis				

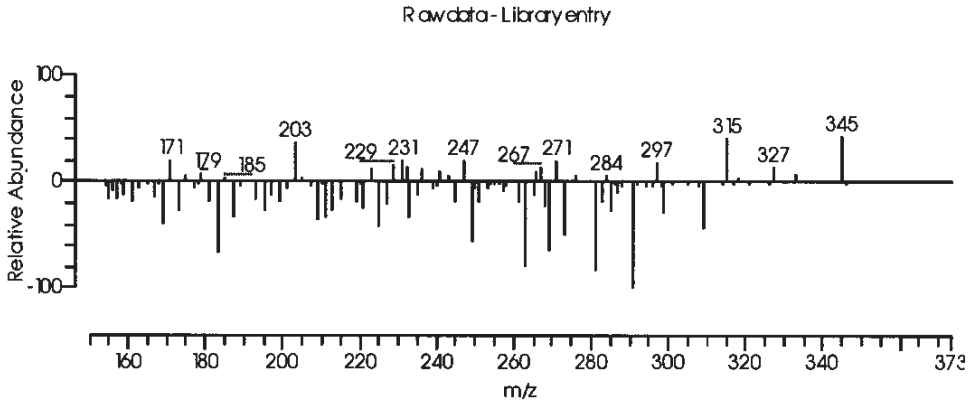
Qualitative Peaks



Spectrum of Raw Data



Difference Spectra



Library Spectrum of Most Probable Hit

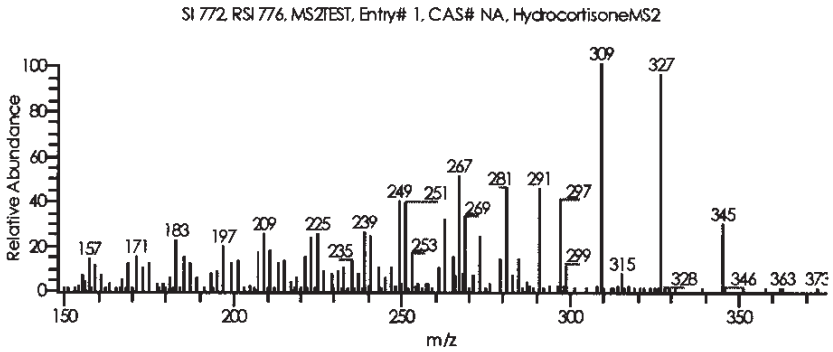
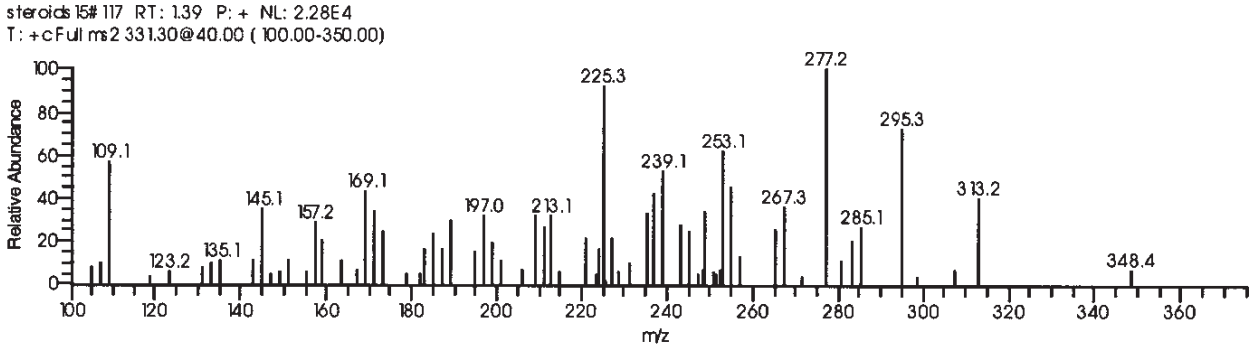


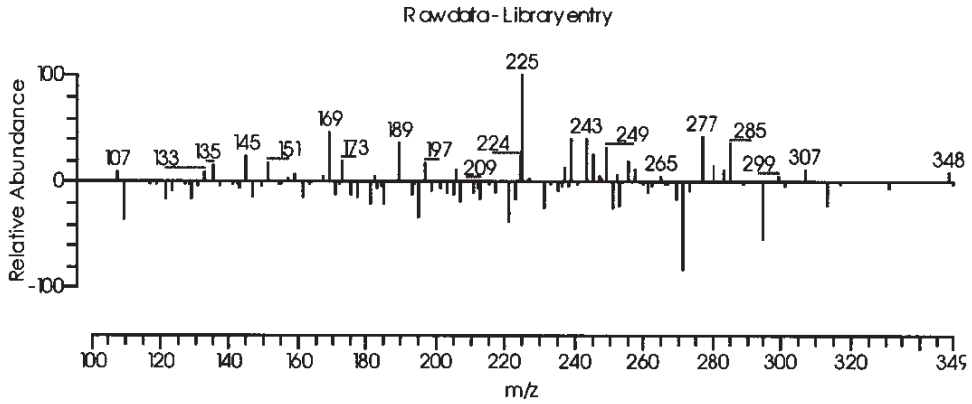
Table of Results

RT	Scan #	Probability, %	Name	SI	RSI	CAS #
0.68	60	98.82	HydrocortisoneMS2	772	776	NA
0.68	60	0.98	ProgesteroneMS2	398	620	NA
0.68	60	0.15	DeoxycorticosteroneMS2	333	482	NA
0.68	60	0.00	MethyltestosteroneMS2	275	437	NA

Spectrum of Raw Data



Difference Spectra



Library Spectrum of Most Probable Hit

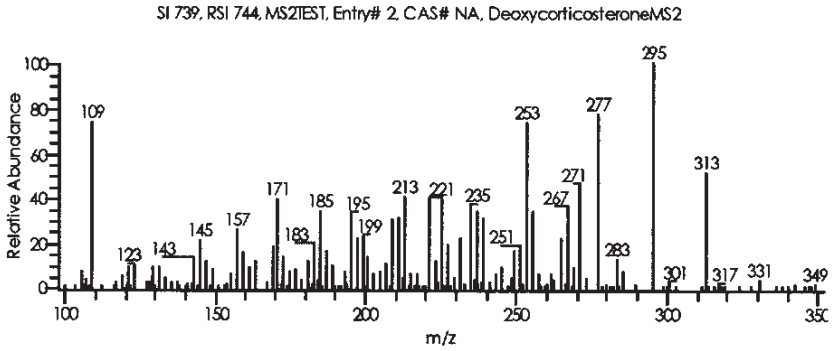
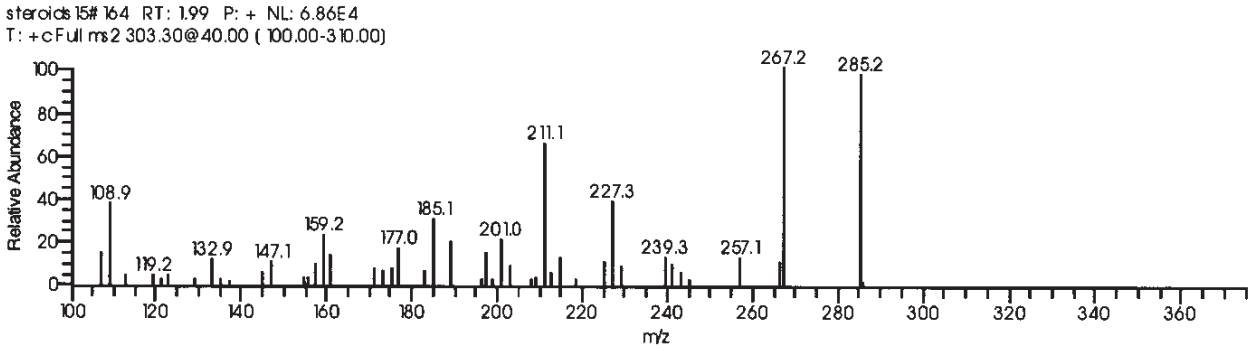


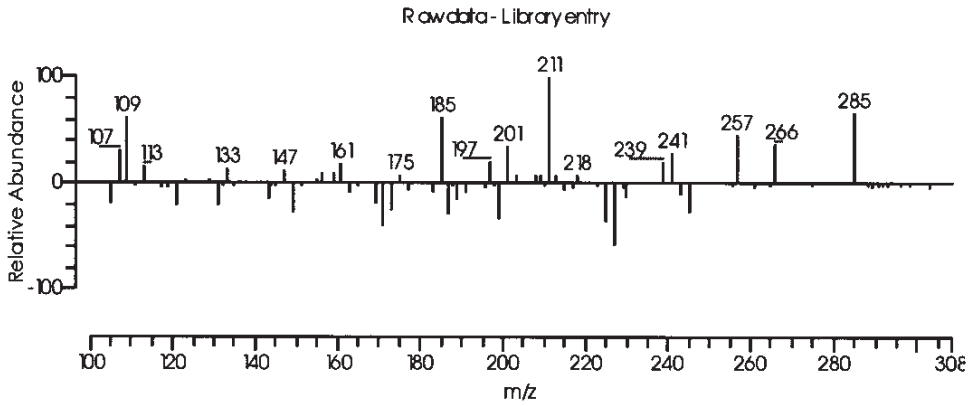
Table of Results

RT	Scan #	Probability, %	Name	SI	RSI	CAS #
1.39	117	98.63	DeoxycorticosteroneMS2	739	744	NA
1.39	117	0.98	MethyltestosteroneMS2	412	563	NA
1.39	117	0.30	ProgesteroneMS2	387	429	NA
1.39	117	0.00	HydrocortisoneMS2	350	395	NA

Spectrum of Raw Data



Difference Spectra



Library Spectrum of Most Probable Hit

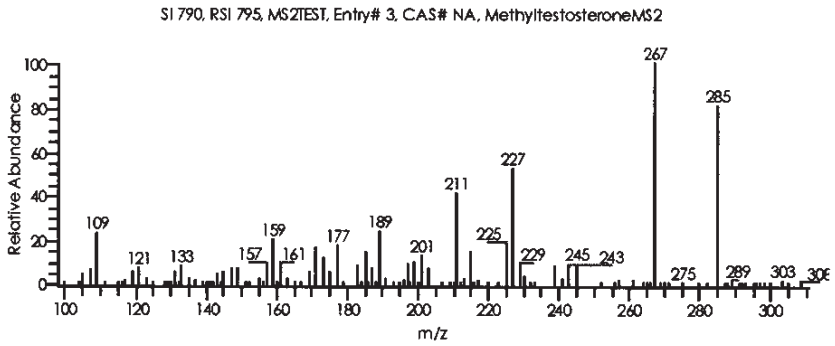
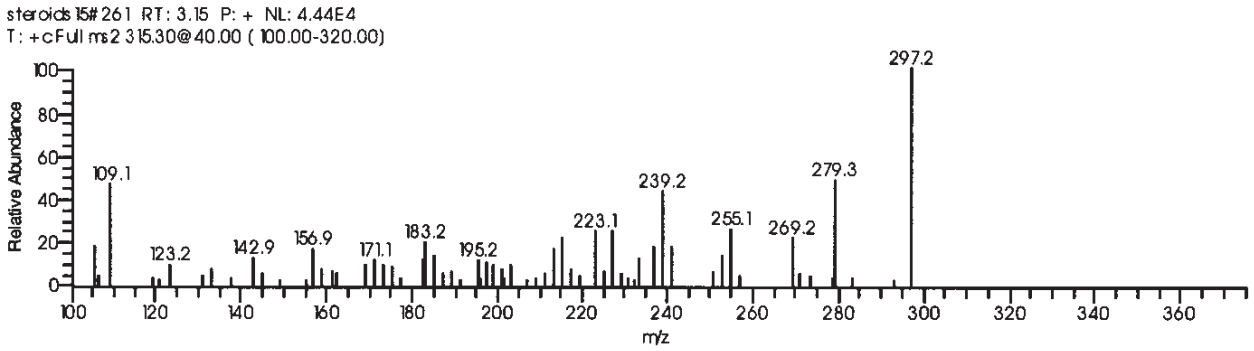


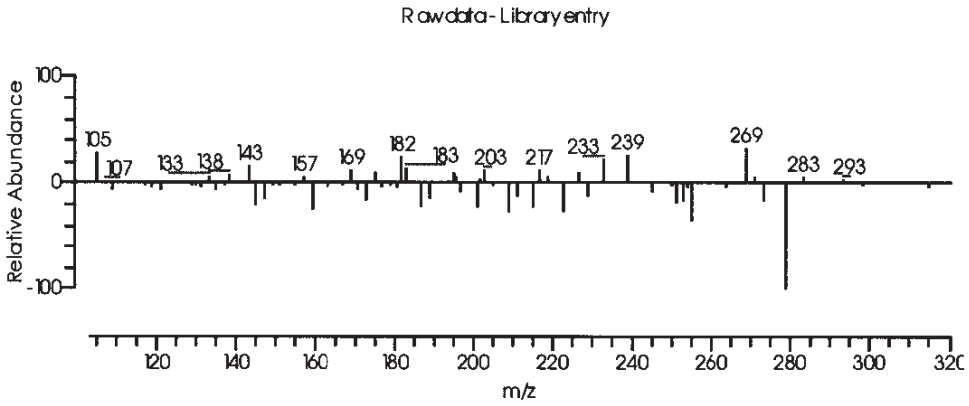
Table of Results

RT	Scan #	Probability, %	Name	SI	RSI	CAS #
1.99	164	98.65	MethyltestosteroneMS2	790	795	NA
1.99	164	0.98	HydrocortisoneMS2	349	349	NA
1.99	164	0.30	DeoxycorticosteroneMS2	324	325	NA
1.99	164	0.00	ProgesteroneMS2	275	369	NA

Spectrum of Raw Data



Difference Spectra



Library Spectrum of Most Probable Hit

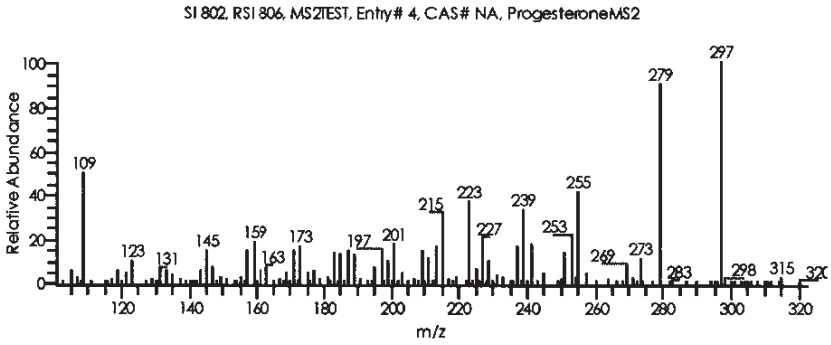


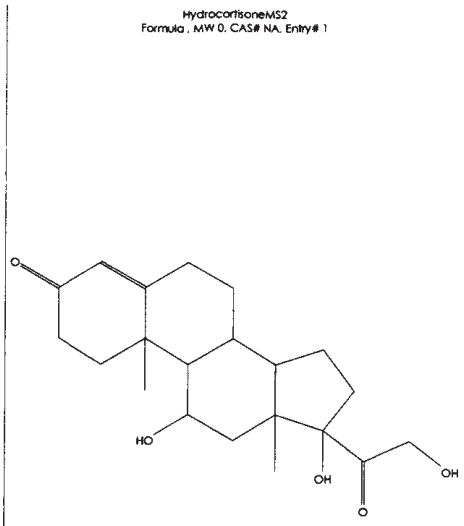
Table of Results

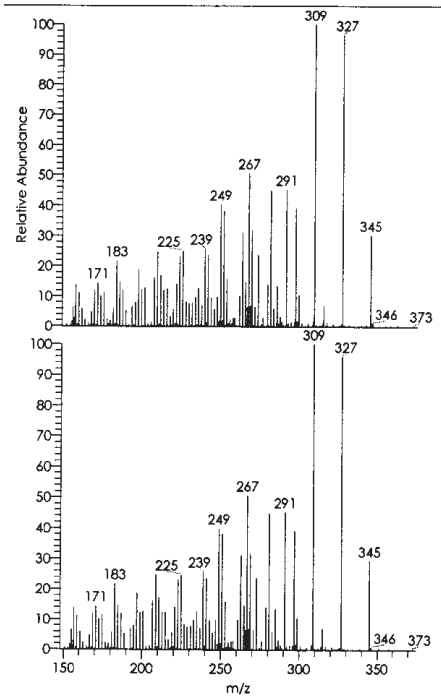
RT	Scan #	Probability, %	Name	SI	RSI	CAS #
3.15	261	98.74	ProgesteroneMS2	802	806	NA
3.15	261	0.98	HydrocortisoneMS2	432	434	NA
3.15	261	0.22	DeoxycorticosteroneMS2	392	488	NA
3.15	261	0.00	MethyltestosteroneMS2	334	377	NA

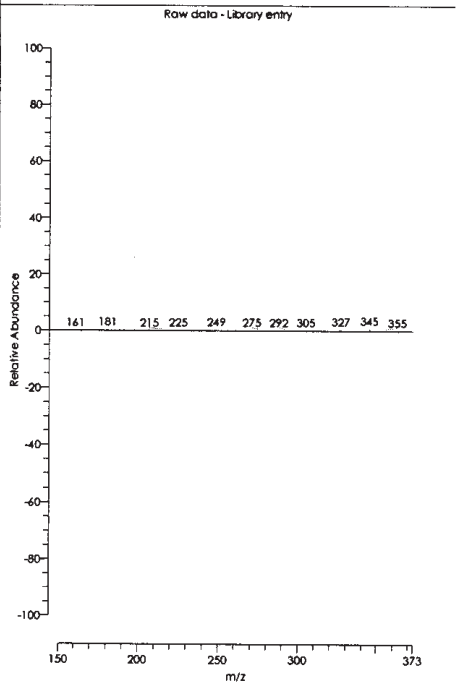
Report from a Library Search Using Qual Browser

The following is an example report of a library search that you can print from Qual Browser.

Hit	SI	RSI	Prob	Name	Library
2	454	651	0.98	Proge	MS2TEST
3	383	523	0.14	Deoxy	MS2TEST
4	343	344	0.03	Hydro	NISTDEMO
5	317	491	0.00	Methy	MS2TEST
6	311	336	0.00	Aldost	NISTDEMO
7	296	303	0.00	Colchi	NISTDEMO
8	282	321	0.00	Folic A	NISTDEMO
9	270	337	0.00	17α-M	NISTDEMO
10	266	555	0.00	Hydro	NISTDEMO
11	266	266	0.00	Reser	NISTDEMO
12	259	306	0.00	Distan	NISTDEMO
13	246	432	0.00	Squal	NISTDEMO
14	244	329	0.00	Ergotc	NISTDEMO
15	244	378	0.00	Diethy	NISTDEMO
16	233	470	0.00	Sulfiso	NISTDEMO
17	232	310	0.00	Octac	NISTDEMO
18	227	305	0.00	Testos	NISTDEMO
19	225	362	0.00	Warfa	NISTDEMO
20	220	293	0.00	Benze	NISTDEMO
21	210	395	0.00	3-Met	NISTDEMO
22	205	530	0.00	1,3-Cy	NISTDEMO
23	200	345	0.00	Chole	NISTDEMO
24	196	275	0.00	Chlorc	NISTDEMO
25	190	521	0.00	Octac	NISTDEMO
26	179	249	0.00	Benze	NISTDEMO
27	178	461	0.00	Benze	NISTDEMO
28	177	353	0.00	Methc	NISTDEMO
29	174	221	0.00	Octat	NISTDEMO
30	169	232	0.00	Triphe	NISTDEMO

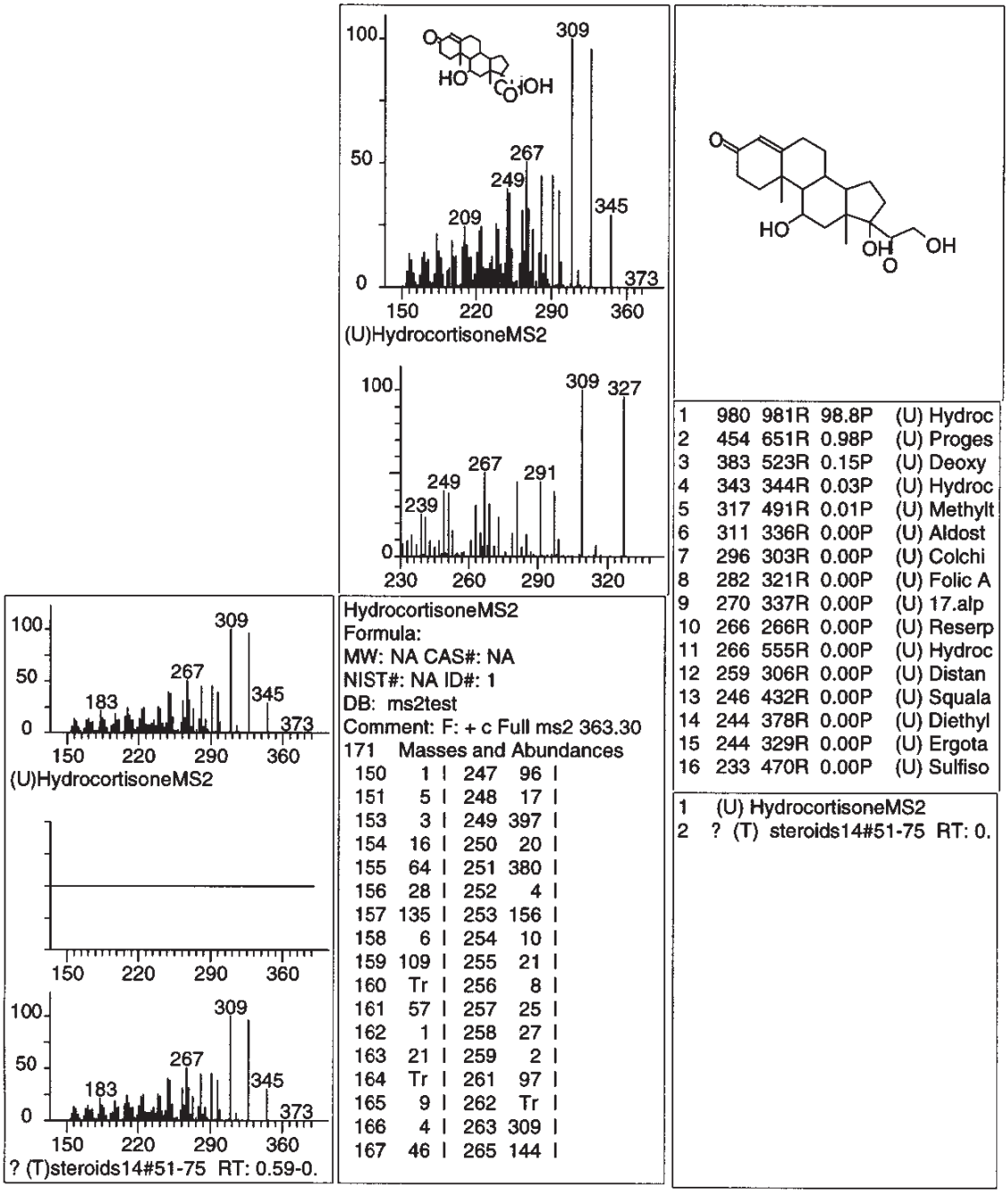






Report from a Library Search Using Library Browser

This section includes an example report of a library search that you can print from Library Browser.



AMDIS Compound Identification

This topic appendix describes using AMDIS to automate compound identification. The Automated Mass Spectral Deconvolution & Identification System (AMDIS) is a computer program developed to reduce the effort involved in identifying compounds by GC/MS while maintaining the level of reliability associated with traditional analysis. AMDIS extracts spectra for individual components from GC/MS data and uses these spectra to identify compounds by matching these spectra with spectra in a reference library.

Contents

- AMDIS Overview
- Automated Compound Identification Using AMDIS

AMDIS Overview

AMDIS uses an extension of the published model peak approach[1] as the basis for the calculations used to extract pure component spectra from complex chromatograms. The model peak approach uses selected ion chromatograms as models for component shape. Based on the shape, individual mass spectral peak abundance profiles are extracted to produce a purified spectrum.

AMDIS was developed at NIST with the support of the Defense Threat Reduction Agency (DOD). NIST reports that the model peak method was successfully used for target compound identification in a large-scale EPA study[2].

The first version of AMDIS was released September 1996, and AMDIS has been distributed at no additional cost along with the NIST Mass Spectral Database since January 1998. AMDIS is included with the Xcalibur software and is also available through the NIST internet site: www.nist.gov/srd/.

[1] Dromey, R. G; Stefi, M. J.; Reindfleisch, T. C; Duffield, A. M. Extraction of Mass Spectra Free of Background and Neighboring Component Contributions from Gas Chromatography/Mass Spectrometry Data. *Anal. Chem.* **1976** *48 (9)* 1368-1375.

[2] Shackelford, W. M.; Cline, D. M.; Faas, L; Kurth, G. An evaluation of Automated Spectrum Matching for Survey Identification of Wastewater Components by Gas Chromatography-Mass Spectrometry. *Analytica Chim. Acta* **1983** *146* 25-27.

Automated Compound Identification Using AMDIS

AMDIS does the following:

- Performs an automated search of the NIST library
- Displays dual chromatographs
- Performs batch analyses
- Builds user defined libraries using either user provided GC/MS files or the NIST Mass Spectral Database
- Provides compound class identification
- Tracks results of routine performance runs
- Uses a library of mass spectra with or without retention indices to identify compounds in a data file

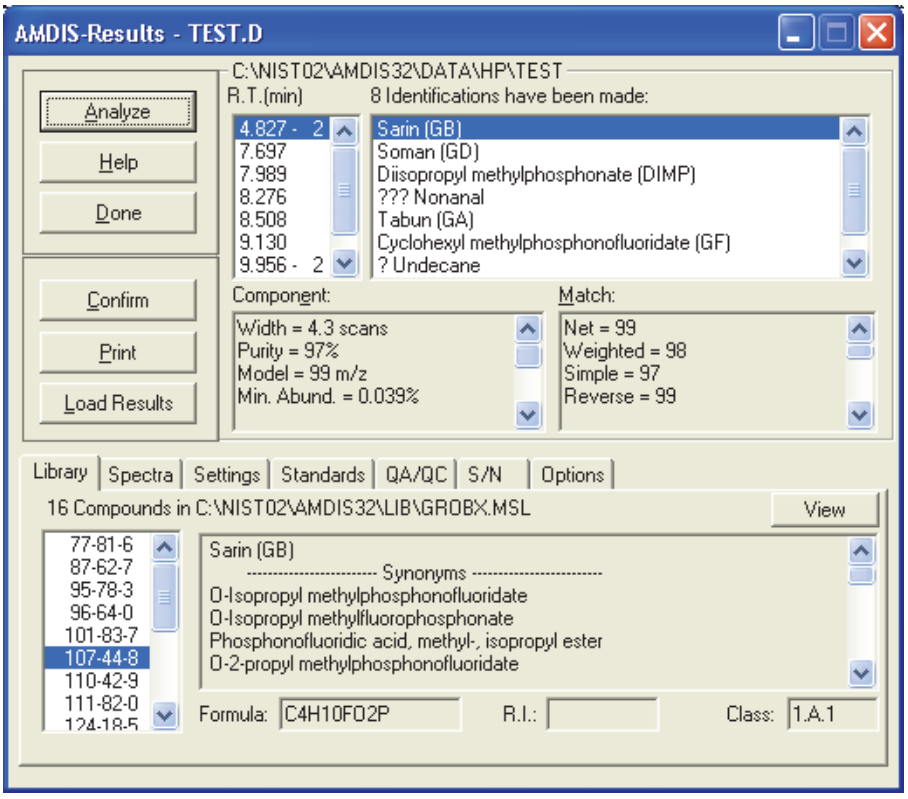
AMDIS has two main windows:

- Results Window
- Confirm Window

Results Window

The Results window contains only search results and is most commonly used for routine analyses (see Figure 72).

Figure 72. AMDIS Results window



The Results window is divided into three areas: the Control panel (top left), the Results pane (top right), and the Library and Settings pane. See Table 1.

Use the Library and Settings pane to

- Examine the library
- Compare the library spectrum with the extracted spectrum
- Examine the settings for the analysis
- View the retention index standards and internal standards
- Examine the QA/QC report or the S/N for the run
- Set options for the printed results

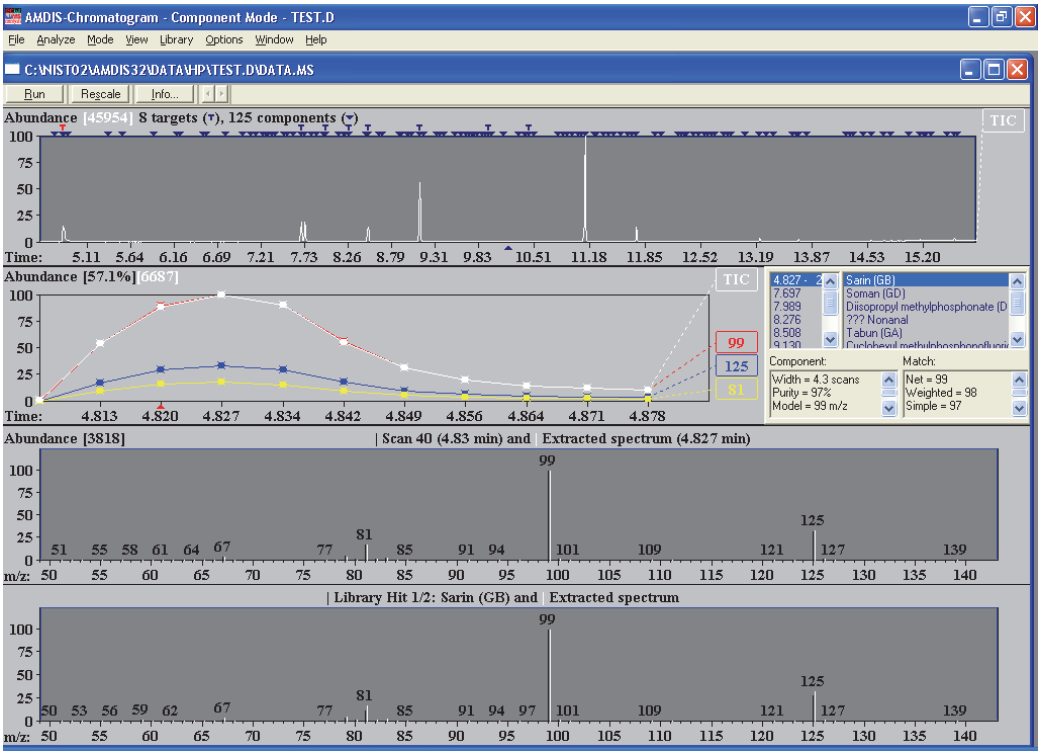
Table 1. Library and Settings pane parameters

Area	Function/options
Control panel (button names)	
Analyze	Open a window to select the type of analysis, the data file to be analyzed, the target library file, and the calibration data or library.
Help	Open Help for the Results window.
Done	Close the window.
Confirm	Open the Confirm window.
Print	Print different reports and information.
Load Results	Select and display the results of a previous analysis.
Results pane (area functions)	
R.T.	View the retention time for each chemical.
N Identifications	View the name of the compound found.
Component	View the component parameters for the deconvoluted chromatographic peak.
Match	View the match factors between the mass spectrum of the component and that of the library.
Library and Settings pane (views)	
Library	Examine the library
Spectra	Compare the library spectrum with the extracted spectrum
Settings	Examine the settings for the analysis
Standards	View the retention index standards and internal standards
QA/QC or S/N	Examine the QA/QC report or the S/N for the run
Options	Set options for the printed results

Confirm Window

The Confirm window shows the data used in identification in more detail than the Results window does (see Figure 73).

Figure 73. AMDIS Confirm window


AMDIS-Chromatogram - Component Mode - TEST.D
File Analyze Mode View Library Options Window Help
C:\NIST02\AMDIS32\DATA\HP\TEST.D\DATA.MS
Run Rescale Info...
Abundance [45954] 8 targets (▼), 125 components (▼)
TIC
Time: 5.11 5.64 6.16 6.69 7.21 7.73 8.26 8.79 9.31 9.83 10.51 11.18 11.85 12.52 13.19 13.87 14.53 15.20
Abundance [57.1%] [6687]
TIC
99
125
81
Time: 4.813 4.820 4.827 4.834 4.842 4.849 4.856 4.864 4.871 4.878
4.827 - 2
7.697
7.989
8.276
8.508
Sarin (GB)
Soman (GD)
Diisopropyl methylphosphonate (D
??? Nonanal
Tabun (GA)
Component:
Match:
Width = 4.3 scans
Purity = 97%
Model = 99 m/z
Net = 99
Weighted = 98
Simple = 97
Abundance [3818]
Scan 40 (4.83 min) and Extracted spectrum (4.827 min)
m/z: 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140
Library Hit 1/2: Sarin (GB) and Extracted spectrum

The Confirm window is divided into the Menu Bar/Button Bar (top), Chromatogram (top most graphical display), Component Profile (middle graphical display), Component/Target Information list (middle numeric display), and Component/Target Mass Spectra (bottom graphical display).

Table 2. Confirm window areas and their functions and options

Area	Function/options
Menu bar	File, Analyze, Mode, View, Library, Options, Window, Help
Toolbar	Run, Rescale, Info, [arrow images]
Chromatogram display	View the ion chromatograms for each ion.
Chromatogram profile	View the total ion current and the largest mass chromatogram peaks over the region actually used in the deconvolution of the component.
Component/Target Information	View either component or target data.
Component/Target Mass Spectra display	View the raw mass spectrum (scan) and the deconvoluted spectrum at a given retention time. Once data has been analyzed, this display also shows the mass spectra of the component and the library.

Library Reference

The Library function in the Xcalibur data system provides different reference windows whose elements are defined here. For information about Library windows, see "Library Browser Windows" on page 4.

Contents

- Library Manager Dialog Box
- Library Search Options Dialog Box
- Spectrum Information Dialog Box
- Library Search Results Window

Library Manager Dialog Box

Use the Library Manager dialog box to manage NIST libraries used with the NIST search software and to convert libraries between the ICIS/GCQ/ITS 40, MassLab, NIST, and ANDI-MS formats.

Xcalibur Library Manager supports the following conversions:

From \ To	ICIS/GCQ/ITS 40	MassLab	ANDI-MS	NIST
ICIS/GCQ/ITS 40		✓	✓	✓
MassLab	✓		✓	✓
ANDI-MS	✓	✓		✓
NIST	✓	✓	✓	

Note The Xcalibur data system does not directly support INCOS, LAB-BASE, or JCAMP library conversions. However, MassLab data system users have a conversion program to convert from a LAB-BASE user library to a MassLab user library. In addition, a conversion tool exists in ICIS (a UNIX system) that can convert a LAB-BASE user library to a MassLab user library.

The Library Manager dialog box has the following pages:

- Convert Libraries Page
- Manage Libraries Page

Convert Libraries Page

Use the Convert Libraries page to convert one type of source library to another type of library at a target location and to copy a library to another location.

Table 3. Convert Libraries page parameters (Sheet 1 of 2)

Parameter	Description
Source Library Details	
Type [Source]	Choose the source library file type that you want to convert to another file type. Select any of the following file types: ICIS/GCQ/ITS 40 (*.lib, .lbr), MassLab (*.idb), ANDI-MS (*.cdf), NIST, or AutoMass (*.spr, *.prs, *.nam, *.hdr).
Library/Browse [Source]	Choose the source library that you want to convert. To change the library, click **Browse** and select the path to the source library on your computer or network.
Process Entries [Source]	Specify the number range of the library entries that you want to convert from the source library. If you leave the box empty, the Xcalibur data system converts all entries. The format is *First Entry-Last Entry*. For example, to convert library entry #100 through library entry #200, type 100-200 in the Process Entries box.
Target library details	
Type [Target]	View the target library file type when converting the source library. If you select source library file type ICIS/GCQ/ITS 40, MassLab, ANDI-MS, or NIST, you can select from the following target library file types: ICIS/GCQ/ITS 40 (*.lib, .lbr), MassLab (*.idb), NIST, or ANDI-MS (*.cdf). If you select source library file type AutoMass, you can only select the NIST target library file type. If you select the library type NIST, the Xcalibur data system displays the path to the NIST library folder in the Library box. You specified this location when you installed NIST.
Library/Browse [Target]	View the file folder to store the converted library file. To change the folder, click **Browse** and select the target folder on your computer or network.
Title [Target]	Type in a title for the ICIS/GCQ/ITS 40 library or for the Mass Lab library that you create during the conversion. You can add a title to the new library using any format. **Note** This box in the Target library details area only becomes active when you select an ICIS/GCQ/ITS 40 or MassLab library.

Table 3. Convert Libraries page parameters (Sheet 2 of 2)

Parameter	Description
Add the library to the NIST software for use with xcalibur	Add the converted library to the NIST software for use with the data system.
Options	
Target library action: Create/Replace	Create a new library in the target directory or to replace an existing library. You can also append (add) the new (converted) entries to a previously created target library.
Target library action: Append	Append (adds) the new (converted) entries to a previously created target library. You can also create a new library in the target directory or to replace an existing library.
Include replicate entries from the NIST library in the target library	Include replicate entries in the target library. Otherwise, leave the box unchecked. **Note** This check box is only active if you are converting from a NIST library to another format.
Replicate library/browse	Specify the location of a replicate library. To change the replicate library, click **Browse** and select the folder for the replicate library on your computer or network. If you specify a replicate library, the Xcalibur data system adds replicate entries into the appropriate replicate library. If you select the library type NIST, the Xcalibur data system displays the path to the NIST replicate library folder in the Library box. You specify this location when you install NIST software.
Button	
Convert	Start the library conversion you have specified using the Convert Libraries page. The data system opens the Library Conversion Status dialog box and displays the Conversion Status progress bar and the Conversion Status box. The Status bar displays messages such as the following: Processed 100% of the entries, continuing on The Conversion Status box displays sequential chronological (top to bottom) messages such as the following: • Started the conversion on SEP 3, 1999 at 10:01, please wait • Finished the conversion on SEP 3, 1999 at 10:02 • Converted 570 entries

Manage Libraries Page

Use the Manage Libraries page to add a library to the NIST libraries list or to delete a library from the NIST libraries list. You can also copy a library to another location.

Table 4. Manage Libraries page parameters (Sheet 1 of 2)

Parameter	Description
NIST Libraries	
NIST Libraries list	View all of the NIST libraries currently available on your computer or network. You can add libraries to this list, delete libraries from this list, and copy libraries on the list to another location.
Buttons	
Add	Add a library to the NIST Libraries list. The Add Library dialog box opens. The Add Library dialog box has the following parameters: • Parameter • Description • Source Use this button to specify the location of the library that you want to add. – Copy the library to the local computer: Select this option to copy the selected library to your computer. – Link to the library from either a remote location or computer: Select this option to access the library remotely. **Note** Because libraries can be large, you might save time by using the Link option rather than the Copy option. Click **OK** when you have selected the library you want to add and selected Action options.
Delete	Delete the library that you have previously selected in the NIST Libraries list. Select the library that you want to delete from the NIST Libraries list. Click **Delete**. The Delete Library message box opens with the following message: Are you sure you want to delete the selected NIST library? Click **Yes**. The Xcalibur data system removes the library from the list.

Table 4. Manage Libraries page parameters (Sheet 2 of 2)

Parameter	Description
Archive	Copy a selected library to another directory on your computer or network. Select the library that you want to copy to another directory. Click **Archive**. The Archive Library dialog box opens. The Archive Library dialog box has the following parameters: • Parameter • Description • Destination: Specify the location for the selected library. Use **Browse** to select a destination for the selected file. Click **OK**. The data system makes a copy of the selected NIST library and stores it in the selected directory.

Library Search Options Dialog Box

Use the Library Search Options dialog box to select and order the libraries used during library searching. You can also change the way that the search is carried out.

The Library Search Options dialog box contains these pages:

- Search Parameters Page
- Libraries Page
- Automation Page
- Limits Page
- Library Search Constraints Page (Library View)

Search Parameters Page

Use the Search Parameters page to select the type of library search, limit the search by a molecular weight constraint, and determine how the results of the search are returned.

Table 5. Search Parameters page parameters (Sheet 1 of 2)

Parameter	Description
Spectrum Search Type	Define the type of library search applied to spectra. There are two main options: Identity and Similarity. The difference between the two search types is primarily in the weightings of the spectrum as a function of mass.
Identity	Apply an Identity search algorithm for library matching of spectra. A Normal Identity search is the default option.
Similarity	Apply a Similarity search algorithm for library matching of spectra.
Normal	Apply a Normal Identity search algorithm for library matching of spectra. This is the default option. A Normal Identity search is suited to low quality or unusual spectra. The search algorithm uses a standard pre-screen search filter.
Quick	Apply a Quick Identity search algorithm for library matching of spectra. Use this option when you are sure the spectrum or compound exists in the library. The search algorithm uses a fast pre-screen search filter.
Spectrum Search Options	
Reverse Search	Specify that the Xcalibur data system sorts matching library spectra (hits) by the Reverse Search Match Factor. By default, the data system sorts search results by the Forward Match Factor.
Penalize Rare Compounds	Reduce the match factors of hit compounds present in few databases. This option is effective only when you have selected one or more of the NIST databases (such as MAINLIB). It has no effect on spectra in user libraries or other commercial libraries. Each reference spectrum in a NIST library contains a record of other commercial databases containing information about the compound. A compound is considered rare if it is present in a limited number of these databases. If you select the Penalize Rare Compounds option, search result compounds present in few or no other databases other than the NIST libraries, will have their match factors reduced (the maximum penalty is 50 out of 1000). This, in effect, leads to a relative increase in the match factors of common compounds, placing them higher in the hit list than exotic isomers with near identical spectra.
Pre-search	
Default	
Off	Turn off the pre-search option.
MW	Restrict the search to library entries with a particular molecular weight. Type the molecular weight in the associated box.

Table 5. Search Parameters page parameters (Sheet 2 of 2)

Parameter	Description
Other Options	
Automation	Indicate whether automatic library searching is enabled.
AutoReport	Print reports of the results of library searching with user spectrum.
Apply Limits	Set limits of *m/z* and peak abundance for spectral comparison.
Use Constraints	Set additional constraints on the search.

Libraries Page

Use the Libraries page to specify the libraries used and the search order for them. It is possible to keep different lists of active libraries for each of the search modes.

Table 6. Libraries page parameters

Parameter	Description
Library Lists	
Available Libraries	List the libraries that are currently excluded from searching during processing. The Xcalibur data system regenerates this list when you open the dialog box.
Included Libraries	List the libraries that are currently included in searches during processing. The order of the libraries defines the order in which they are searched by the data system.
Buttons	
Remove	Transfer a library from the Selected Libraries list to the Available Libraries list.
Up	Move a library in the Selected Libraries list up one position (earlier in the search order).
Down	Move a library in the Selected Libraries list down one position (later in the search order).

Automation Page

Use the Automation page to specify values for an automated library search.

Table 7. Automation page parameters

Parameter	Description
Number of hits to print	Set the number of spectra to be printed per page. The default value of 2 prints the unknown and the top two matches on a single sheet of paper.
Include spectrum plot in report	Include spectrum, text of intensities, and masses in report.
Draw structure in plots	Add a molecular structure to the spectrum plot, if this is available.
Apply maximum spectrum length	Provide an upper mass limit for printed spectrum.
Return focus to caller upon completion	Used in the context of an instrument control program calling the search program.
Automatic search on	Carry out a library search automatically in Library Browser when a spectrum is exported from Qual Browser.

Limits Page

Use the Limits page to define limits for a library search.

Table 8. Limits page parameters

Parameter	Description
Apply limits	Apply limits to the library search.
Minimum Abundance	Specify the minimum level of abundance before including in a search.
Minimum m/z	Specify the minimum level of abundance before excluding from a search.
Maximum m/z	Specify the maximum level of abundance before excluding from a search.
Set Default	Set parameter values as the default for future searches.

Library Search Constraints Page (Library View)

Use the Constraints page to define additional constraints on the search. For example, limit the search to only compounds with names containing specified letters (such as “ol” for alcohols), or specify that only certain elements can be present in the compound.

Limit a library search to increase processing efficiency. For example, you might want to exclude certain high intensity ions that appear in many compounds or that are present in the spectrum background. You can target a search to a particular range of molecular weights or to compounds containing certain elements. This view is available both in the Library Browser and the Qual Browser.

Table 9. Library Search Constraints Page parameters (Sheet 1 of 7)

Parameter	Description
Molecular Weight	
☑	Limit the library search to compounds with a specific molecular weight or molecular weight range by selecting the Molecular Weight Enable check box.
Range	Type a molecular weight or molecular weight range in the box (for example, 200-250). During a search, the Xcalibur data system only compares processed spectra with reference data derived from compounds with a molecular weight within the specified range.
Name Fragment	
☑	Limit the library search to compounds with a specific name or name fragment by selecting the Name Fragment Enable check box.
Name	Type a text string (up to 39 characters) to represent a fragment of a compound name; for example, “cyclo”. During the library search, the Xcalibur data system filters search results and only returns those containing the specified text in their names. The entry is not case sensitive, so “CYCLO” returns compounds containing the fragments “cyclo”, “Cyclo” and “CYCLO”.

Table 9. Library Search Constraints Page parameters (Sheet 2 of 7)

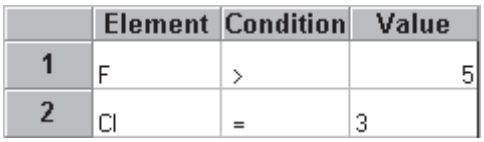
Parameter	Description
Elements Value	
Individual Element Table	Set specific criteria about the elements required in a library hit. Each row in the table represents an element constraint.  There are three parts to each constraint: • **Element**: An IUPAC-approved abbreviation for an element, for example "Cl" for chlorine • **Condition**: A mathematical operator, < (less than), > (greater than), or = (equals) • **Value**: A numerical value representing the number of atoms of the specified element required to satisfy the constraint. In the example shown here, the Xcalibur data system only returns search results for compounds that contain more than five fluorine atoms or exactly three chlorine atoms. You do not need to provide a complete elemental profile. The library search returns compounds if they satisfy all the specified criteria regardless of any other elements present.
[Row Number]	Enter a new item in the last unused row in the table (indicated by an asterisk). Each numbered row represents an item in the table.
Element	Type the IUPAC-approved abbreviation for the element you want to use an element constraint. It is used in conjunction with the Condition list and Value box in the same row within the Individual Element table. To enter an element constraint, click the box and type the required abbreviation. For example, to apply carbon as an element constraint, type "C". The data system adds a new row to the table for further entries.
Condition	Enter a condition for an element constraint in this box. The Xcalibur data system uses this condition in conjunction with the Condition list and Value box in the same row within the Individual Element table. Valid conditions are: < (less than) > (greater than) = (equals) To type an element constraint condition, click the box to activate the list. Click the down arrow and select the required abbreviation.

Table 9. Library Search Constraints Page parameters (Sheet 3 of 7)

Parameter	Description
Value	Type a numerical value for an element constraint in this box. The data system uses this value in conjunction with the Condition list and Value box in the same row within the Individual Element table.The value represents the number of atoms of the specified element required by library compounds to satisfy the constraint. To type an element constraint value, click the box and type the required number (the valid range is 0 to 99).
Elements Present	
☑	Select to constrain the library search to compounds containing specific elements using the Individual Element or Elements in Compound methods. You can use the two types of elemental constraints together, but make sure there are no contradictions. For example, you might put “C=0” in the Individual Element group and then list “C” in the Elements in Compound box. When a contradiction occurs, a warning dialog box opens.
Elements In Compound	
Elements	Specify a list of elements that must be present in search results. To enter an element list, click the box and type the IUPAC-approved abbreviation for each element. Separate each element in the list (of up to 30 characters) by a comma.
All	Specify that the Xcalibur data system should return search results containing all, and only, the listed elements. For example “C, H, O” would return HCHO but not CO2, CH4, or CH2Cl2. Compare these results with the Some option.
Some	Specify that the Xcalibur data system return search results that contain at least one of the specified elements and no elements that are unlisted. For example, “C, H, O” would return CO2, CH4, HCHO but not CH2Cl2. Compare these results with the All option.
Clear	Delete the text in the Elements in Compounds box.

Table 9. Library Search Constraints Page parameters (Sheet 4 of 7)

Parameter	Description
Mass Spectral Peak Constraints	
☑	Build a profile of ions and ion abundances to be matched against library entries during the search. The search algorithm only returns search results matching the specified constraints.
Mass spectral peak constraints table	Set specific criteria about the mass spectral peaks required in a library hit. Each row in the table represents an individual mass spectral peak constraint. There are four components to each constraint represented by the table columns: **Type**: Normal, Loss, Rank, or Maxmass ***m/z***: In a Normal, Rank, or Maxmass type constraint, use this box to type the *m/z* value of the mass spectral peak to limit. In a Loss type constraint, use this box to type the value of a neutral loss. **From**: In a Normal, Loss, or Maxmass type constraint, type the minimum abundance of the constrained mass spectral peak in this box. In a Rank type constraint, type the lowest position of the ion in an intensity ordered list of spectral peaks in this box. **To**: In a Normal, Loss, or Maxmass type constraint, type the maximum abundance of the constrained mass spectral peak in this box. In a Rank type constraint, type the highest position of the ion in an intensity ordered list of spectral peaks in this box.
[Row Number]	Enter a new item in the last unused row in the table, indicated with an asterisk. Each numbered row represents an item in the table.

Table 9. Library Search Constraints Page parameters (Sheet 5 of 7)

Parameter	Description
Type	Specify the type of ion constraint. **Normal**: Applies to a specific ion represented by its *m/z* value. The From and To values represent the abundance of the ion. **Loss**: Describes a neutral loss from a molecular ion. In this case, the *m/z* value (limited to 64) represents the mass of the 'lost' neutral group, for example, for methyl *m/z* = 15. For this constraint to be matched, a library spectrum must contain the following: • A fragment ion at an *m/z* value 15 less than the molecular ion • An abundance in the specified From and To range **Rank**: Tests the order of an ion in the spectrum in terms of relative abundance. Ions are ranked from the largest (the base peak) to the 16th. A compound matches a Rank constraint if its library spectrum contains a mass spectral peak with these criteria: • At the specified *m/z* value • Ranked between the specified From and To rank positions If you specify the same number in both fields, the designated ion must have that rank in the retrieved spectrum. **Maxmass**: Sets a constraint on the *m/z* value of the most significant high mass ion. Library search results must feature the following: • An ion at the specified *m/z* value • No significantly larger masses at higher *m/z* values. • An abundance in the specified From and To range
m/z	In a Normal, Rank, or Maxmass type constraint, type the *m/z* value of the mass spectral peak to be constrained in this box. The data system discards a library hit if it does not contain a mass spectral peak at the specified *m/z* value. In a Loss type constraint, use this box to type the value of a neutral loss. The application discards a library hit if it does not feature a fragment ion at an *m/z* value appropriate to the specified neutral loss (in relation to the molecular ion).

Table 9. Library Search Constraints Page parameters (Sheet 6 of 7)

Parameter	Description
From	In a Normal, Loss, or Maxmass type constraint, type the minimum abundance of the constrained mass spectral peak in this box. In a Rank type constraint, you use this box to type the lowest position of the ion in an intensity ordered list of spectral peaks. You can specify the same number in both From and To boxes. In this case, the Xcalibur data system discards a library hit unless the designated mass spectral peak is present in exactly the specified abundance or rank in the retrieved spectrum.
To	In a Normal, Loss, or Maxmass type constraint, type the maximum abundance of the constrained mass spectral peak in this box. In a Rank type constraint, type the highest position of the ion in an intensity ordered list of spectral peaks in this box. You can specify the same number in both From and To boxes. In this case, the Xcalibur data system discards a library hit unless the designated mass spectral peak is present in exactly the specified abundance or rank in the retrieved spectrum.
Absolute	Specify how the Xcalibur data system applies the From and To parameters in the Mass Spectral Peak Constraints table. Select the **Absolute** option if you want the application to evaluate all table entries as a percentage of the base (largest) ion in the spectrum. Values must be between 0 and 100%. For example, if you type 10 and 50 in the From and To fields of a Normal type constraint, the application discards any search results in which the specified mass spectral peak is not present at an abundance of between 10 and 50%. In the case of Normal and Loss type constraints, the abundance values can also be Relative.
Relative	Specify how the Xcalibur data system applies the From and To parameters in the Mass Spectral Peak Constraints table. Select the **Relative** option if you want the application to treat the first entry as an absolute Normal or Loss type. The application considers subsequent entries in the table relative to the first. In the following example, library search results must contain the following: • An ion at *m/z* 125 with an abundance between 10 and 50% of the base ion • An ion at *m/z* 250 with an intensity between 50% and 999% of the observed intensity of the first ion in the list • Relative mode is not available for Rank or Maxmass types.

Table 9. Library Search Constraints Page parameters (Sheet 7 of 7)

Parameter	Description
Other Databases	**Selection Criteria**
☑	Limit the library search to entries in the NIST library also featured in other databases. Each entry in the NIST library contains a list of other commercial databases containing information about the compound. The data system reports search results featuring in one or more of the selected databases (a hit does not have to feature in all the selected databases).
Fine	Report search results from reference compounds or spectra also to be found in the commercially available Fine Chemical Index.
TSCA	Report search results from reference compounds or spectra also to be found in the Toxic Substances Control Act Inventory (TSCA).
RTECS	Report search results from reference compounds or spectra also to be found in the Registry of Toxic Effects of Chemical Substances (RTECS).
EPA	Report search results from reference compounds or spectra also to be found in the Environmental Protection Agency (EPA) Environmental Monitoring Methods Index.
USP	Report search results from reference compounds or spectra also to be found in the US Pharmacopoeia (USP)/U.S.A.N.
HODOC	Report search results from reference compounds or spectra also to be found in the CRC Handbook of Data of Organic Compounds (HODOC).
NIH	Report search results from reference compounds or spectra also to be found in the NIH-NCI Inventory File.
EINECS	Report search results from reference compounds or spectra also to be found in the European Index of Commercial Chemical Substances (EINECS).
IR	Report search results from reference compounds or spectra also to be found in the NIST/EPA Gas Phase IR Database.
Clear All	Clear all the check boxes in the Other Databases area.
Button	
Save As Default	Validate and save the settings on the current page as default settings. The data system uses these settings for all new processing methods, overriding the previous default values permanently.

Spectrum Information Dialog Box

Use the Spectrum Information dialog box to type or to change information stored with a library spectrum. The dialog box displays information for the spectrum selected in the Spec List in the Librarian window.

Figure 74. Spectrum Information dialog box

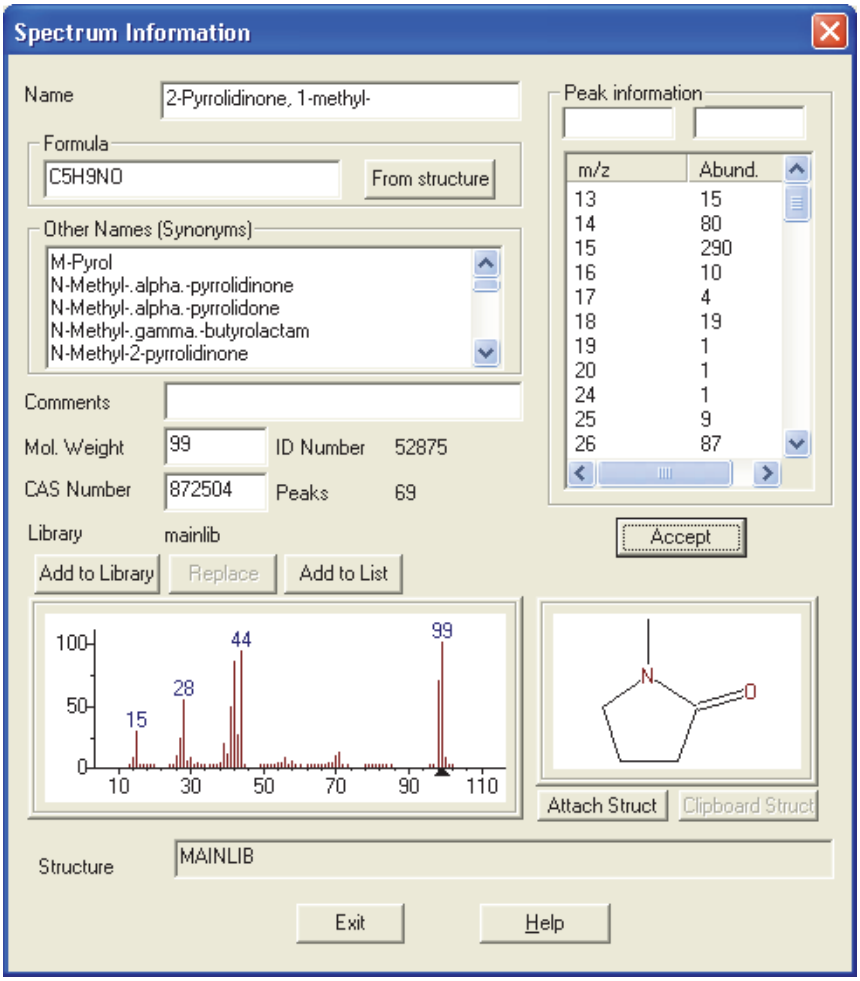


Table 10. Spectrum Information dialog box parameters (Sheet 1 of 2)

Parameters	Action
Name	Type a name for the spectrum.
Formula	Type the chemical formula, for example, C12H8Cl6O.
Other Names	Type synonyms for the compound.
Comments	Type any comments about the spectrum.
Mol. Weight	NIST MS Search assigns a molecular weight based on the formula. If no formula is available, type the molecular weight.
ID Number	View the ID number assigned to the library entry.

Table 10. Spectrum Information dialog box parameters (Sheet 2 of 2)

Parameters	Action
CAS Number	View the CAS number for the compound. (You need not enter this information.)
Peaks	View the number of peaks in the mass list.
Buttons	
Add to Library	Add the edited spectrum and structure to an existing or new library.
Replace	Replace the spectrum in the library from which it came.
Add to List	Add the edited spectrum to the Spec List.
Attach Struct	Obtain a structure from other libraries.
Clipboard Struct	Attach a structure from the clipboard, if present.

To edit the mass list, use the Peaks Info area.

Library Search Results Window

Qual Browser displays this window in its workspace when you submit a spectrum in a Spectrum View to a library search or when you open a result file containing library search results from qualitative processing.

The Library Search Results window displays matching library spectra (hits) in a four-pane arrangement. Clockwise from the top left, the four panes are as follows:

Hit List

The Hit List lists the best matches found during the library search. Three factors describe the accuracy of the match to your spectrum:

SI A direct matching factor for the unknown and the library spectrum.

RSI A reverse search matching factor ignoring any peaks in the unknown that are not in the library spectrum.

Prob A probability factor based on the differences between adjacent hits in an SI ordered list.

With the SI and RSI matching factors, a perfect match results in a value of 1000. As a general guide 900 or greater is an excellent match; 800-900, a good match; and 700-800, a fair match. A matching factor less than 600 is a poor match. Unknown spectra with many peaks tend to yield lower match factors than otherwise similar spectra with fewer peaks.

The probability factor is a complex parameter based on the SI matching factor and the difference between adjacent matches. If a hit has an SI match factor > 900 and the next best hit has a match factor of 300, the probability of the compound being correctly identified is high. Conversely, if several hits are returned with very similar SI matching factors, the probability of a correct assignment is low.

Molecular Structure

Shows the formula, structure, molecular weight, name and library index number of the currently selected hit in the Hit List.

Difference Spectrum

Compares the submitted spectrum with the currently selected library spectrum in the Hit List. Peaks above the X-axis are relatively more intense in the sample than the library entry. Negative peaks are relatively more intense in the library entry than in the sample spectrum.

Comparison

Displays the submitted spectrum above the currently selected library spectrum in the Hit List.

Note Avoid making positive assignments based solely on the statistical result of a library search. The Xcalibur data system might identify a compound with an unusual structure (or, more importantly, an unusual mass spectrum) in a definitive way. More usually, your unknown might be a member of a class of compounds with very similar mass spectra. The ability of Qual Browser or any search system to distinguish between them is limited. In many cases, the best that the search algorithm can do is identify a class of compounds that have similar mass spectra — and usually similar structure. In most cases, you should seek confirmation by other analysis techniques.

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